PREFACE

This annual report is published every year to provide individuals and organizations, interested in R&D related to the chemical industry, with a document that tracks the progress made by projects supported through the Department of Energy's (DOE's) Office of Industrial Technologies. The report describes, in essence, a portfolio of investments. The **Introduction** provides background information on DOE, the Office of Energy Efficiency and Renewable Energy, the Office of Industrial Technologies, and the Chemical Industry Team. The project reviews that follow are grouped by level of application to activities or materials associated with chemicals or the chemical industry. The first section, **Chemical Industry Team (CIT) Projects**, contains reviews on projects supported directly from the team's budget. The **OIT Chemical Industry Projects** derive financial support from other Office of Industrial Technologies team budgets but are also technologies that are of major interest to the chemical industry. Other projects included in this annual portfolio are **DOE's Environmental Technology Partnerships**, which focus on helping industry move from a clean-up and waste management focus to a pollution prevention strategy, and a listing of OIT technologies that have been commercialized and are of relevance to the chemical industry.

As we strive to continue the progress made by the team this year, we welcome your comments, thoughts and suggestions. On overall team matters please contact the CIT leader, Bruce Cranford, at Bruce.Cranford@hq.doe.gov or at the U.S. Department of Energy, Office of Industrial Technologies, 1000 Independence Avenue SW, Washington, DC 20585. For comments or inquiries on the specific projects included in this annual report please see the point of contact listed with each project. Additional information on the CIT is available on the World Wide Web (http://www.oit.doe.gov/IOF/chemicals). Current members of CIT include:

- David Boron
- Bruce Cranford
- Simon Friedrich
- Amy Manheim
- Charles Russomanno

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INTRODUCTION

The U.S. Department of Energy: Energy Efficiency and Renewable Energy

The U.S. Department of Energy (DOE) contributes to the health and prosperity of the Nation by providing the scientific foundation, technology, policy, and institutional leadership necessary to achieve efficiency in energy use, diversity in energy resources, productivity in industry, sustainability for our communities and our environment, and ample employment opportunities in our competitive economy. Within the DOE, the Office of Energy Efficiency and Renewable Energy forms collaborations and cost-shared partnerships with external clients in the manufacturing, buildings, transportation, and utility sectors. This approach to leveraging the Department's federal funds with private funds and sharing information produces tangible benefits that save energy, preserve the environment, and encourage economic growth.

AUTHORITY

The Federal role in pursuing industrial sector R&D is well established, having been mandated by legislation authorizing programs for energy conservation, first within the Federal Energy Administration (FEA), and later within the Energy Research and Development Agency (ERDA) and DOE. Formerly known as the Office of Industrial Programs, OIT has been involved in efforts to improve industrial energy efficiency since the passage of the Federal Non-Nuclear Energy Research and Development Act in 1974. Under this Act, DOE is authorized to "advance energy conservation technologies, including -- but not limited to -- productive use of waste, including garbage, sewage, agricultural waste and industrial waste heat; reuse and recycling of material and consumer products." In 1975, the Energy Policy and Conservation Act called for Federal support to increase the energy efficiency of U.S. industry, particularly the most energy-intensive industries.

NATIONAL ENERGY POLICY ACT

The Energy Policy Act (EPAct) of 1992 (Public Law 102-486) authorizes programs in the following areas: Sections 2101 (General Improved Energy Efficiency), Section 2107 (Improved Efficiency in Energy-Intensive Industries), and Section 2108 (Energy Efficient Environmental Program).

The Office of Industrial Technologies: Collaborating with Industry on Technology Solutions

In 1994, U.S. industry, including manufacturing, agriculture, mining, and construction, accounted for 1.7 trillion dollars of the economy's gross product (24%) and employed over 27 million people. In manufacturing alone, its 380,000 facilities accounted for nearly 1.2 trillion dollars of the economy's gross product. Today, U.S. industry faces serious energy, economic, and environmental challenges that affect domestic and international competitiveness as well as the potential for continued industry growth.

Within the DOE's broader mission, **the Office of Industrial Technologies (OIT)** strives to meet future energy, environment, and economic challenges and promote a strong industrial base by developing technology-based solutions in partnership with U.S. industry. The OIT's programs are designed to share the cost of development, demonstration, and deployment of technologies to increase energy efficiency, reduce waste, improve productivity, and enhance environmental performance for the most energy and waste intensive industries in the United States.

The OIT's strategies for achieving these goals are to:

- Conduct cost-shared R&D that addresses high-priority opportunities for advanced process technologies identified through and driven by industry-formulated visions in the forest products and paper, steel, aluminum, metal casting, chemicals, petroleum refining, and glass industries;
- Conduct R&D on generic, longer-term, high-risk material and component technologies with applications across industrial sectors;
- Identify and prioritize opportunities for developing "leapfrog," energy- and materials-efficient, pollution-preventing technologies through government-industry R&D partnerships;
- Team with industry, states, and the U.S. Environmental Protection Agency to provide cost-sharing for projects to showcase innovative applications of energy- and waste-reducing technologies in a commercial setting;

- Develop strategic alliances with other DOE organizations; federal, state, and local governments; trade groups; and industry to leverage funds to develop and deploy energy-efficient and pollution-preventing technologies in industry;
- Team with other federal agencies, industry trade organizations, industrial firms, and public interest groups to identify and establish voluntary targets and government incentives for pollution prevention and to develop a scientific basis for regulatory frameworks;
- Provide technical assistance and information to accelerate technology deployment; and
- Use awards, "seals of approval," and other market stimulation techniques to encourage innovation and bold investment decision-making in industry.

Extensive private industry involvement is an essential element of OIT programs, and industrial cost-sharing is required for all R&D. Generally, industrial cost-sharing increases as the technology advances (see Figure 1). National laboratories and universities also collaborate with private industry on OIT programs. Mechanisms for **industry/national laboratory collaboration** include sharing information (no cost), joint programs with no funds exchanged, joint programs with a third party, "work for others" arrangements, full-cost recovery with user facilities, consortia, and cooperative research and development agreements (CRADAs). A similar approach involves **government/industry/university procurement mechanisms** for doing business, such as financial assistance, cooperative agreements, grants, and cost-shared contracts.

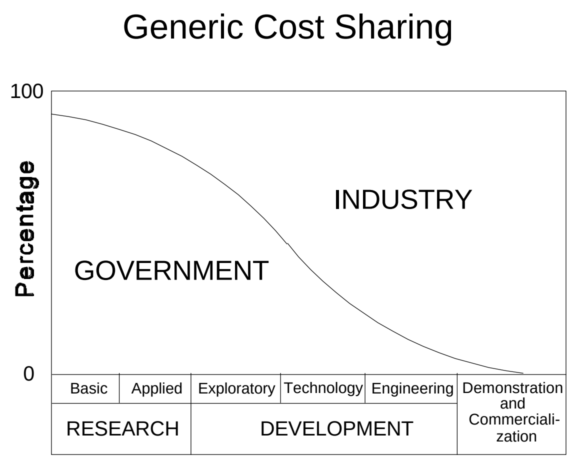


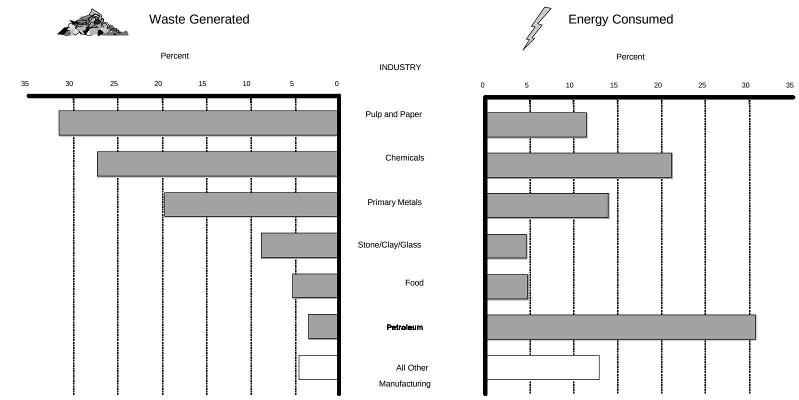
Figure 1. Industrial Cost Sharing

The OIT solicits ideas for new technology R&D from industry, universities, national laboratories, and the environmental research community. Proposals are acquired through competitive solicitations, unsolicited submissions, and industrial/national laboratory collaboration. Proposals submitted to the OIT are evaluated to determine whether they fall within OIT's priority R&D areas and must also address the following five criteria: energy savings; waste reduction, utilization, or conversion; economic attractiveness; industrial support; and demonstrated need for government funds. Projects with a need for government funding generally involve a high degree of technical risk, benefits that contribute to the national welfare and are not exclusive to a single company, efforts beyond the ability of a single firm or industry, a long-term payback, and/or direct cooperation between the OIT and industry. High-priority R&D needs are identified through the Industries of the Future process.

Under its **Industries of the Future (IOF)** process, the OIT encourages collaboration among companies in the most energy- and waste-intensive manufacturing industries and facilitates a process in which each industry develops a strategic vision of its own desired future. In addition, the industry plots out a course to develop technology or a "roadmap" to achieving its vision. This process enables each industry to identify and prioritize its collective technology needs in the context of the market, business, social, and regulatory drivers affecting that industry.

The identification of the technology critical to the needs of industry enables the OIT and other government R&D providers to focus their limited funding and other resources in the most important areas. The OIT industry teams draw on these visions to create their R&D project portfolios. The result is an R&D agenda that is highly effective in addressing an industry's very diverse technology needs. Clearly this visioning effort promotes leveraging of scarce public and private sector R&D resources by building R&D partnerships among government, industry, national laboratories, and universities.

In keeping with its energy efficiency mission, the OIT concentrates the IOF process on industries that offer the best opportunities for saving energy and reducing waste. These industries -- known as the materials and process industries -- include the **chemical**, **petroleum refining**, **forest and paper products**, **steel**, **aluminum**, **metal casting**, and **glass** industries. These seven industries account for about 80% of U.S. manufacturing energy consumption, about 80% of the volume of all waste and pollution generated in manufacturing, and nearly two-thirds of all pollution control expenditures in manufacturing (see Figure 2). The energy costs for these industries range from about 5% to 65% of total operating costs — greatly exceeding the manufacturing average of about 3%. Collectively, these seven industries also account for about one-seventh of all U.S. merchandise trade and their continued survival is essential to the continued competitiveness of the U.S. economy.



Sources: *Manufacturing Consumption of Energy 1991*; EIA. *National Biennial RCRA Hazardous Waste Report 1989*; EPA.
Report to Congress: Solid Waste Disposal in the United States; EPA 1988.

Figure 2. Waste Generation and Energy Consumption in the Materials and Process Industries (Percent of Manufacturing Total)

The Chemical Industry Team (CIT): Supporting the Chemical Industry's Needs into the 21st Century

The OIT **Chemical Industry Team (CIT)** continues OIT's mission of creating partnerships among industry, trade groups, government agencies, and other organizations to research, develop, and deliver advanced energy efficiency, renewable energy, and pollution prevention technologies for the chemical industry. These advanced technologies will help the chemical industry to save energy and cut waste, lower operating costs, boost productivity, and prevent pollution.

In partnership with companies like Air Products and Chemicals, General Motors, Union Carbide, and Dow Chemical, CIT members managed research, development, scale-up, and deployment projects in alternative feedstocks, separations, biocatalysis and bioprocessing, and waste recycling and utilization worth more than $13 million. With successful development and anticipated industry acceptance, by the year 2010 these technologies could annually reduce U.S. industry's energy use by nearly 0.5 quadrillion Btu, reduce costs by nearly $10 billion, eliminate 10 million metric tons of carbon equivalent emissions, and eliminate 17 million metric tons of other wastes. In addition, the CIT works closely with the Laboratory Coordinating Council (LCC). Created in 1995 by DOE national laboratories, the LCC facilitates collaboration with and within the chemical industry and helps industry to access the laboratories' capabilities.

THE CHEMICAL INDUSTRY

In the United States the chemical industry employed about 825,000 people in 1994 and had production valued at over $333 billion, including $49 billion in exports. This industry is exceptionally large and diverse, producing over 60,000 different products ranging from basic commodity chemicals to mass-marketed consumer goods such as drugs, detergents, and paints. The chemical industry is also the second largest industrial consumer of energy and the largest generator of regulated industrial waste in the United States. As a result, many opportunities exist to improve the industry's energy efficiency and reduce its generation of waste. The chemical industry's lead in technology development contributes to its enormous success in global markets. To maintain its competitiveness, the industry increasingly has shifted its R&D toward new product development at the expense of innovations to improve process efficiency. In addition, the growing list of environmental regulations is taking an increasing share of chemical industry investment capital as firms rush to meet deadlines for emissions standards with end-of-pipe controls rather than develop more environmentally sound technologies.

In December 1996, a number of organizations representing the chemical industry produced a report articulating the chemical industry's needs as it enters the 21st century. ***Technology Vision 2020: The U.S. Chemical Industry*** was developed through a joint effort of the American Chemical Society, the American Institute of Chemical Engineers, the Chemical Manufacturers Association, the Council for Chemical Research, and the Synthetic Organic Chemicals Manufacturers Association. The report provides a technology vision and establishes technical priorities in areas critical to improving the chemical industry's competitiveness; develops recommendations to strengthen cooperation among industry, government, and academia; and provides direction for continuous improvement through step-change technology. *Technology Vision*

2020 also assesses the chemical industry's technology needs in four areas: new chemical science and engineering technology, supply chain management, information systems, and manufacturing and operations. The report outlines five broad goals that the industry must achieve over the next 25 years:

- Improved operations, with a focus on better management of the supply chain;
- Improved efficiency in the use of raw materials, the reuse of recycled materials, and the generation and use of energy;
- A continued leadership role in balancing environmental and economic considerations;
- An aggressive commitment to longer term investment in R&D; and
- Balanced investments in technology achieved by leveraging the capabilities of government, academia, and the chemical industry as a whole through targeted collaborative R&D efforts.

The CIT team has accomplished much over the past year in addition to supporting the chemical industry's visioning process. **CIT Highlights for 1996** include continuing to help industry articulate its strategic vision in technology "roadmaps." These roadmaps will identify technical pathways from current technologies to the advanced technologies needed to achieve the vision; and will serve as the basis for setting priorities and establishing the industry's research agenda. The CIT has also been busy establishing and maintaining numerous R&D partnerships with companies, universities, and other organizations located across the country. This year the CIT projects involved almost 100 working partnerships in over 30 states (see Appendix A).

In addition, over the past several years CIT-supported projects have resulted in a number of commercialized technologies (see Appendix B). In 1996, the CIT saw the completion and commercialization of the "Scrap Tire Recycling" project. This effort developed a new surface treatment for finely ground tire rubber that can be used to manufacture high value composites that, in turn, replace petroleum-derived polymers. This newly treated material greatly increases wheel traction on wet surfaces and will put some of the 70 million scrap tires sent to stockpiles each year to good use.

CIT members and project partners have also been active presenting and publishing many technical papers, chapters, and books. For example, papers and reports have appeared in *Applied Environmental Microbiology*, *Protein Engineering*, *Nature Biotechnology*, *Biotechnology and Bioengineering*, *Journal of the American Chemical Society*, *Inorganic Chemistry*, *Journal of Physical Chemistry*, *Chemical Processing*, *Studies in Surface Science and Catalysis*, *Journal of Catalysis*, *Journal of Chemical Physics*, *Physical Review*, and *Industrial Engineering Chemical Research*. Book chapters authored by CIT partners include "Recycling of Polymers," in Conversion and Utilization of Waste Materials, and "Surface Modified Rubber Particles for Polyurethanes," in Handbook of Additives. In addition, patents were filed for rubber compositions and solvent resistant microorganisms, several software programs were created, and a number of site demonstrations were completed. For a comprehensive listing of accomplishments, see the Highlights section for each project.

OFFICE OF INDUSTRIAL TECHNOLOGIES
Productivity through Technology

Advanced Bioprocessing Concepts

BACKGROUND

Immobilized cell systems that allow the properties of biocatalysts to be determined and bioreactors to be developed for optimum use in multi-phase systems.

Bioreactors may be applied to the continuous production of industrial products such as enzymes and chemicals. This project will advance the practical and fundamental knowledge of bioreactor dynamics and immobilized biocatalyst systems. Specifically the project will develop and test new bioreactor configurations; model the kinetic properties of biocatalyst particles and the dynamics of bioreactor systems; and develop enhanced bioreactors for continuous production of industrial products. The project emphasizes multi-phase reactors. However, the multi-phase emphasis will move away from pure aqueous systems to nonaqueous bioprocessing, including liquid organic-phase bioreactors and gas phase bioreactors.

PROJECT HIGHLIGHTS FOR FY 1996

- Immobilization and reactor design for the dehalogenation of process byproducts are being investigated. Dehalogenation addresses a direct industrial need to transform a current byproduct waste of organic synthesis for recycle in the process. The project team has produced the enzyme using an improved organism developed by Dow. Several modes of immobilization have been tested, including a successful immobilization in a porous glass.

- Experimental and modeling tasks have begun in the areas of interfacial phenomena and contacting schemes using enzymes in organic media and in gas-phase reactors.

- A vocabulary was developed with appropriate definitions and symbol representation to simplify classification of enzymatic reactions in nonaqueous biocatalysis. In conjunction with the derivation of this terminology, a technology roadmap was constructed that can be used to rank the priority of issues associated with work that has been and will be performed in this field.

- Bioprocessing concepts are being investigated for conversion of sparingly soluble gaseous substrates. Current research employs trickling filter bioreactors for the degradation and subsequent removal of gaseous alkanes (pentane and isobutane) from effluent air streams. Advances in this technology hold promise for providing low-cost alternatives to more traditional, energy intensive treatment methods such as incineration and adsorption. Experiments were concluded in three experimental degradation systems; development efforts in gas-phase bioreactors using biofilters have also been concluded. These techniques are now being extended to gaseous substrates with biocatalysts in an organic phase to improve reaction and product solubility.

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Advanced Distillation Control Techniques

BACKGROUND

A comparison of advanced distillation control techniques that gives industry the information needed to run distillation columns more energy efficiently, reducing energy consumption by an average of 15%.

Distillation in the refining and chemical industries consumes 3% of the total U.S. energy use (Humphrey et al., 1991), which amounts to approximately 2.4 quadrillion Btu of energy annually. In addition, distillation columns usually determine the quality of final products and many times determine the maximum production rates.

Distillation columns are often over-refluxed to ensure that the product purity specifications are met. That is, more energy than necessary is used to meet the product specifications. As a result, industry many times uses 30% to 50% more energy than necessary to produce its products. It has been estimated that an overall average 15% reduction of distillation energy consumption can be attained if better column controls are applied (Humphrey et al., 1991).

Industry does not have a consistent basis upon which to compare the various options for distillation control. Since distillation controls are not fully understood, they may be applied where not needed or not applied where needed.

Under this project, detailed simulations will be performed of a range of distillation columns with varying degrees of control difficulty to assess the control performance of various control options. A range of column designs and operating conditions will be studied.

ENERGY SAVINGS AND ENVIRONMENTAL BENEFITS

By the year 2010, the use of this technology will provide the following annual benefits:

- 288 trillion Btu of energy savings
- 19 million tons of CO_2 emissions avoided.

This estimate of energy savings is based on the overall average energy savings of 15% (Humphrey, et al., 1991), 80% market penetration, and an energy mix of 10% oil, 70% gas, and 20% coal.

PROJECT HIGHLIGHTS FOR FY 1996

- Advanced control methods were applied to a Dow Chemical industrial C3 splitter resulting in $500,000 per year in savings from reduced energy use.
- Papers were published comparing conventional and advanced control for the base case design of the C3 splitter.
- A method was identified to evaluate the variability of impurities in products as a means of comparing controller performance.
- The effects of distillation column reboiler and accumulator liquid holdup on controller performance were identified.

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OFFICE OF INDUSTRIAL TECHNOLOGIES
Productivity through Technology

Advanced Electrodialysis Processes for Separations and Pollution Prevention

BACKGROUND

An advanced electrodialysis technology that will recycle byproduct wastes and provide replacements for toxic solvents.

Many waste streams generated during industrial process operations are both economic and environmental burdens. Some of these streams in the chemical, pharmaceutical, and pulp and paper industries contain salts (contaminated with organics) that can be recovered through the novel application of advanced electrodialysis technologies.

Argonne National Laboratory (ANL) is working with NTEC EDSep., Inc. and U.S. Filter, Inc. to develop, demonstrate, and commercialize advanced electrodialysis applications in the process industries. In addition, ANL is developing a novel and low cost process called direct esterification that will produce lactate ester. Lactate ester can replace large volumes of chlorinated and other toxic industrial solvents that are used in a wide variety of industries. ANL and NTEC EDSep., Inc. are performing process integration, scale-up, and commercialization activities for the novel lactate ester production process.

ENERGY SAVINGS AND ENVIRONMENTAL BENEFITS

By the year 2010, the use of this technology will provide the following annual benefits:

- 77 trillion Btu of energy savings
- 2.7 million tons of salt waste avoided
- 9.9 million tons of carbohydrate waste avoided
- 0.5 million tons of toxic waste avoided.

PROJECT HIGHLIGHTS FOR FY 1996

- Laboratory development for several applications of the advanced electrodialysis technologies was successfully completed. One application is proceeding to the in-plant pilot phase.
- The reaction mechanisms of the direct esterification process were elucidated and an approach was developed to improve product yield.
- Three U.S. patent applications were filed for the advanced electrodialysis technologies, the novel esterification process, and another membrane separation process.
- CogniTek has licensed and, with a major food products manufacturer, is commercializing the polylactic acid technology developed by ANL for food applications. The two companies have formed a Cooperative R&D Agreement (CRADA) with the U.S. Department of Agriculture to test their applications.
- NTEC EDSep., Inc. is developing a partnership with companies from the agriprocessing and solvent manufacturing industries to commercialize the first generation lactate ester technology.
- U.S. Patent Number 5,464,760, "Fermentation and Recovery Process for Lactic Acid Production," was issued. S.P. Tsai, S.Y. Moon, and R. Coleman, November 7, 1995.
- Datta, R. and S.P. Tsai. "Technology and Economic Assessment of Lactic Acid Production and Uses." Presented at the Corn Utilization Conference VI, St. Louis, Missouri, June 4-6, 1996.
- Datta, R. and S.P. Tsai. "Electrodialysis Separation Processes for Waste Recycle and Reuse in Process Industries." Presented at the AIChE 1996 Spring National Meeting, New Orleans, Louisiana, February 25-29, 1996.

PARTICIPANTS/PARTNERS

ANL, NTEC EdSep., Inc. (a CRADA partner), U.S. Filter, Inc., and CogniTek.

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AIChE-CWRT Cooperative Agreement

BACKGROUND

A program of collaborative research and development in pollution prevention that reduces waste, transfers technology to industry, and educates the public about pollution prevention.

The Center for Waste Reduction Technologies (CWRT), a division of the American Institute of Chemical Engineers, has over 20 member companies doing industry-sponsored research to develop innovative waste reduction technologies and methodologies. Together with the DOE, the CWRT is working to reduce the generation of waste, improve productivity, and enhance the environmental performance of processes in U.S. industry. Under a cooperative agreement signed in 1994, the DOE and CWRT support cost-shared, pre-competitive R&D projects, with an emphasis on research that can serve as a basis for subsequent development of commercial technologies. The cooperative agreement also supports technology transfer, information dissemination, and education by developing engineering curricula and providing workshops and seminars for industry.

In 1996, four projects were being conducted under the DOE-CWRT cooperative agreement:

- Novel Reactor Design;
- Separations Technology Tools for Clean Process Advisory Systems;
- Chemical Precipitation and Recovery of Ammonia and Amines; and
- Emerging Separation Technologies and Separative Reactors Workshop.

PROJECT HIGHLIGHTS FOR FY 1996

- Phase I of the Novel Reactor Design Collaborative Research Project was completed. Consortium members Monsanto, Eastman Chemical, Air Products and Chemicals, Olin Chemical, Rhone-Poulenc, and SRI are proceeding with design and development for the final phase of the work. A patent was issued to SRI International for the reactor process.
- The DOE approved a proposal to sponsor a workshop on "Emerging Industrial Separations Technology" to develop technology roadmaps in support of the chemical industry's vision, *Technology Vision 2020*.
- A proposal, "Total Cost Accounting: The Development of a Validated Computing Tool for Use in the Chemical and Pharmaceutical Industries," was developed by the CWRT and submitted for DOE approval.

PARTICIPANTS/PARTNERS

CWRT members are as follows: 3M, Air Products and Chemicals, AM-RE Services, Argonne National Laboratory, Arthur D. Little, Battelle Pacific Northwest National Laboratory, B.F. Goodrich, CH^2M Hill, Dow Chemical, Eastman Chemical, the Electric Power Research Institute, General Electric, Hoechst Celanese, ICI Americas, Los Alamos National Laboratory, M.W. Kellogg, Kinetics Technology International, Merck & Co., Monsanto, Nofsinger, Inc. (a division of Burns and McDonnell), Rhone Poulenc North America, Rohm and Haas, SmithKline Beecham, SRI International, Union Carbide, the U.S. DOE, and the U.S. Environmental Protection Agency.

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Biocatalysis by Design

BACKGROUND

Development of tools for atomic scale modeling and simulation of biological systems applied to develop biological catalysts for industrial processes.

Prediction of the three dimensional structure of molecules is important for drug design and other biotechnology applications. Tools are needed for modeling and simulation of biological systems and for the prediction of critical parameters for experimental validation of the models. These tools may be applied to overcome barriers to the widespread application of biotechnology in industry.

This project seeks to develop tools for atomic scale modeling and simulation of biological systems and to predict critical parameters for experimental validation of the models. Methods and techniques for predicting the structure and function of proteins are under investigation, with the goal of designing proteins that recognize specific DNA sequences. These proteins will be used to develop regulatory proteins for controlling biocatalysts.

PROJECT HIGHLIGHTS FOR FY 1996

Protein Folding from Primary Sequence. The project team is using the hierarchical strategy for predicting protein tertiary folding from primary sequence data. Quantum mechanical calculations are being used to optimize parameters for tripeptides. Further quantum mechanics work is proceeding on the side-chain interactions and hydrogen bonding to the backbone.

Dynamics of Protein Folding. It is assumed that all natural proteins will fold to their thermodynamic minimum. Existence of certain mutants opens opportunities for designing proteins that can fold faster and in higher yields. The formation of an alpha-helix from polyalanine has been simulated. These results provide the first data concerning the conditions leading to helix formation. The data are being analyzed for patterns that might suggest experimental tests of these simulations.

Force Field Development for Nucleic Acids and Proteins. The new force field for nucleic acids implements an accurate hydrogen bond interaction between the bases. The project team now has an excellent description of structure and energetics for the Guanine-Cysteine pair and for the structure of the Adenine-Thymine pair. Protein force field development is partially complete.

Copper Proteins: Transfer and Electronic Structure. Density Functional Theory (DFT) calculations were done for the Cu(I)/Cu(I) state of the simplified $(Cu)_2(SCH_3)_2(NH_3)_2$ model with C_1 symmetry. The results indicate that the two highest occupied orbitals lie very close together but are well separated from the next level. These results support the interpretation that the CuA center has a rapid rate of electron spin relaxation.

PARTICIPANTS/PARTNERS

The California Institute of Technology (CalTech), Aramco, Oronite, Chevron, Asahi Chemical, Hughes, Hercules, XEROX, BP Chemical, AlliedSignal, and IBM.

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Biological/Chemical Caprolactam Process

BACKGROUND

A new biomanufacturing process for making caprolactone, an alternative feedstock for Nylon-6, that creates little or no waste, uses 50% less energy, and costs only half as much as methods used to make caprolactam, from which Nylon-6 is currently made.

Nylon-6 is currently produced from caprolactam. The chemical synthesis of caprolactam from cumene is a complex, multi-step process that is energy intensive and generates considerable waste. Nylon-6 could also be produced from caprolactone. However, the current market price for caprolactone makes this route uneconomical.

A laboratory-demonstrated biological process has been developed that would provide a one-step, cost-effective production process for caprolactam manufacture that requires 50% less energy than the current process, costs half as much (considering both capital and energy costs), and produces almost no waste byproducts.

This project sought to establish the technical feasibility of the biomanufacturing process for converting inexpensive cyclohexane into caprolactone. Under this project, the feasibility of the laboratory-demonstrated biomanufacturing process was established, and the process is now available to be optimized for possible scale-up to pilot plant scale.

ENERGY SAVINGS AND ENVIRONMENTAL BENEFITS

By the year 2020, the use of this technology can provide the following annual benefits over the use of the previously-existing technology:

- 12 trillion Btu of energy savings
- 14,000 tons of waste production avoided (ammonium sulfate, acetone, phenol, and cumene)
- 800,000 tons of CO_2 emissions avoided.

The biological process works at ambient temperature and pressure and produces only water and carbon dioxide as byproducts. (The carbon dioxide will be captured for other uses.)

PROJECT HIGHLIGHTS FOR FY 1996

- The final project report was completed.
- St. Martin, E.J. 1996. *A Biological/Chemical Process for Reduced Waste and Energy Consumption Caprolactam Production*. DOE/AL/94462-2. Report prepared by AlliedSignal, Inc. for the U.S. Department of Energy, Washington, DC.

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Clean Fractionation of Wood for Cellulose-Based Fibers and Films

BACKGROUND

A process that reduces the amount of coproducts from the pulping operation to negligible levels with a resulting product that does not require chlorine bleaching.

This project will demonstrate a clean fractionation process based on organic solvents that separates biomass feedstocks into their component fractions with zero or near zero cross-contamination from coproducts (lignin and hemicellulose). This clean separation results in a product that can be used as chemical grade cellulose for conversion into a cellulose derivative and can subsequently be bleached with peroxide rather than chlorine.

Markets for high quality cellulose produced by organic solvent-based clean fractionation include rayon and acetate fibers for apparel, curtains, and drapery; thermoplastics for tool handles, toys, automotive parts, etc.; cellulose acetate films used in laminate boards, photographic films, and surface coatings for wood finishes; cellulose ethers used in food thickeners and stabilizers, latex paints, and drilling muds; and cellophane. Other commercial, organic solvent-based processes have not achieved sufficient product quality to penetrate all of these markets

ENERGY SAVINGS AND ENVIRONMENTAL BENEFITS

By the year 2010, the use of this technology will provide the following annual benefits:

- 10.4 trillion Btu of energy savings
- 0.14 million tons of waste production avoided.

PROJECT HIGHLIGHTS FOR FY 1996

The large scale fractionation reactor continues to be used extensively to compare the effects of scale-up of the process on the performance parameters of the cellulose fraction. Reproducibility between the large scale and smaller scale fractionations is excellent, and the physical properties of the cellulose are comparable between the different fractionation scales. Physical properties of concern are viscosity (a measure of the relative strengths of the cellulose chains — higher is better) and kappa (a measure of the amount of residual lignin that is present — lower is better). A new pretreatment of the wood feedstock has been developed. Large scale fractionation of the pretreated feedstock gave a cellulose fraction with the highest viscosity observed to date for runs in our larger reactor. The results from this run may indicate an improvement in conditions that will lead to higher viscosities in general. Work continues on sorting out the effects of the pretreatment from other reaction parameters.

Work has also been carried out in developing a methodology for the isolation of the hemicellulose material from clean fractionation. The hemicellulose fraction is important because it could serve as a chemical feedstock for materials not available from the cellulose fraction. Ion exchange chromatography has been found to be a useful method for this process. This treatment allows solvent removal and isolation of products without decomposition, a problem in earlier attempts to purify the hemicellulose fraction. This purification has the added benefit of removing any metal ions that may have been present in the starting feedstock sample, or leached from the reactor during fractionation. These ions are a problem because they tend to interfere with work-up and analysis.

PARTICIPANTS/PARTNERS

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Computer-Aided Molecular Design of Biomimetic Catalysts

BACKGROUND

Computer-aided design methodologies developed and applied to construct biomimetic catalysts for use in the conversion of carbon dioxide to products.

Carbon dioxide (CO_2) is a renewable resource that may be used as a feedstock for industrial processes and clean fuels. In addition, CO_2 is a greenhouse gas; its use as a feedstock can help reduce greenhouse gas emissions to the atmosphere.

The project will develop Computer-Aided Molecular Design (CAMD) methodologies and apply them to the design of biomimetic catalysts that activate and convert CO_2. The current focus is on the design of a catalyst to convert CO_2 to anhydrous formaldehyde. The ultimate goal of the research is a process for solar-driven reduction of CO_2.

Application of the biomimetic CAMD methodology, coupled with experimental studies of the designed catalysts, is providing the knowledge base on structure-reactivity relationships needed for the design of catalysts tailored for specific reactions.

ENERGY SAVINGS AND ENVIRONMENTAL BENEFITS

Global warming resulting from the greenhouse effect has given new impetus to chemical storage of solar energy. Further, CO_2 conversion using solar or electrochemical energy would provide a renewable source of clean fuels and feedstocks.

PROJECT HIGHLIGHTS FOR FY 1996

- *Catalyst Testing.* The testing program is focusing on CO_2 conversion for fuel cell electrodes instead of CO_2 reactions.

- *Synthesis of Advanced Catalyst Designs*. New cobalt-porphyrin catalysts have been synthesized. The testing results indicate that these porphyrins give improved current-voltage properties in commercial gas-diffusion electrodes.

- *Structural Characterization and Validation of the CAMD Methods.* A computational procedure for normal structural decomposition has been developed and implemented.

- Jentzen, W., I. Turswska-Tyrk, W.R. Scheidt, and J.A. Shelnutt. 1996. "Solid-State and Solution Structures of (Porphinato)nickel(II) Are Planar by X-ray Diffraction and Resonance Raman Spectroscopy." *Inorg. Chem.*, **35**: 3559-3567.

- Jentzen, W., E. Unger, G. Karvounis, J.A. Shelnutt, W. Dreybrodt, and Reinhard Schweitzer-Stenner. 1996. "Conformational Properties of Nickel(II)Octaethylporphyrin in Solution. 1. Resonance Raman Profiles and Temperature Dependence of Structure-Sensitive Raman Lines." *J. Phys. Chem.*, **100**: 14184-14191.

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Electroplating Waste Minimization

BACKGROUND

The development of a membrane-based technology, Polymer Filtration, that merges ultrafiltration with specially designed metal-binding water soluble polymers to treat electroplating rinse water, eliminating sludge production and saving energy.

There are approximately 10,000 electroplating facilities in the Unites States, each of which produces an average of 55,000 gallons per day of wastewater requiring treatment to remove toxic metal ions. About 90% of the water comes from rinsing operations. The treatment of this wastewater converts the toxic metal wastes to large quantities of hydroxide sludges that are sent to land disposal. New advanced metal separations are needed by private industry, the DOE, and the Department of Defense to aid compliance with regulatory restrictions and to improve process economics, conserve resources, and minimize wastes.

This project is developing new separations technologies for metal ions. For treating dilute metal-ion mixtures, smaller point-source treatment units used in conjunction with plating line segregation expend less energy than end-of-pipe treatment systems. By focusing on the point source, the chemistry of metal separations can be optimized for the particular plating line, thereby optimizing the removal and recovery of the metal ions of interest. The polymer filtration technology developed under this project merges ultrafiltration with specially designed metal-binding water soluble polymers. This technology eliminates sludge production, saves energy, and discharges water that is even cleaner than required by Environmental Protection Agency regulations. Recovered metal ions are returned to the electroplating process, reducing raw materials costs.

ENERGY SAVINGS AND ENVIRONMENTAL BENEFITS

By the year 2010, the use of this technology will provide the following annual benefits:

- 27 trillion Btu of energy savings
- 249,000 tons of hazardous sludge production avoided.

Industrial benefits include reduced industrial liability, the ability to meet current and proposed regulations for discharged metals, and reduced raw material costs.

PROJECT HIGHLIGHTS FOR FY 1996

- A successful pilot demonstration was held with MicroSet at State Plating in Indiana.
- The project received the Industrial Partnership Office's 1996 Award for Excellence in Industrial Partnerships.
- The project received the 1995 Los Alamos National Laboratory (LANL) "Director's Very Large Team" Distinguished Performance Award.
- A license agreement was finalized with Academy Corporation.
- Smith, B.F., M. Cournoyer, B. Duran, D. Ford, R. Gibson, M. Lin, A. Meck, P. Robinson, and T. Robison. 1996. "Chelating Water-Soluble Polymers for Waste Minimization." Report Number LA-UR-95-3224.

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Environmental Process Design Modeling

BACKGROUND

Production of computer-assisted tools that allow industrial processes to be designed so as to prevent pollution, thereby economically reducing waste generation and energy use over the life cycle of a facility.

Between 250 and 750 million tons of industrial hazardous wastes are generated each year, with the bulk of this generated by the chemical process industries. This project will develop computer-aided tools for process design that will minimize both waste generation and energy use.

ENERGY SAVINGS AND ENVIRONMENTAL BENEFITS

By the year 2010, the use of this technology will provide the following annual benefits:

- 50 trillion Btu of energy savings
- 10 million tons of hazardous waste eliminated.

PROJECT HIGHLIGHTS FOR FY 1996

- The software is being developed and tested as modules.

- *Pollution Assessment Module (PAM):* A case study of cogeneration facilities was conducted on the PAM. The study showed that process economics alone are not adequate to describe the competitiveness of energy technologies; the full assessment must include environmental aspects.

- *Safety Index Generator:* Correct safety considerations for a Natural Gas Liquids plant were predicted by the test index generator. The technology is to be certified by Dow Chemical.

- *Pollution Evaluation Index Generator:* A prototype was tested by modeling a cogeneration facility; local and global effects of emissions were analyzed.

- *Pollution Prevention Module:* The technical program for pollution prevention in process design has begun, with a subcontract to the Pacific Northwest National Laboratory.

- Shonnard, D.R. et. al. 1996. "Pollution Assessment Software as Chemical Industry Software Enhancements." *Proc. 5th World Congress of Chemical Engineering*, San Diego, CA.

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Enzyme Catalysts for a Biotechnology-Based Chemical Industry

BACKGROUND

Enzyme catalysts that are developed based on design rules for enzymes at the level of their amino acid sequences to improve stability and catalytic activity in polar nonaqueous solvents.

Improved understanding of the molecular basis of protein stability and enzyme catalysis, combined with the ability to create large quantities of proteins of virtually any amino acid sequence, gives us the ability to redesign natural proteins to fit the requirements of industrial applications. As a result, biotechnologists no longer have to limit themselves to designing processes around natural biocatalysts — designing a biocatalyst to fit the process is gradually becoming an achievable goal. The ability to carry out biochemical syntheses in organic solvents, where solubilities are greatly enhanced and new chemistries are available, greatly expands the scope and potential applications of biocatalysis in the chemical industry.

This research will provide general tools and design rules for engineering stable and efficient biological catalysts. Strategies employed by this project are to use both random and site-directed mutagenesis techniques to alter the amino acid sequence of Subtilisin E, a serine protease with numerous potential applications in organic synthesis and preparation of novel polymers. Research will investigate reaction conditions essential in maintaining the activity of enzymes in extreme environments. The investigations will study enzyme stability and reactivity in water-miscible organic media and determine the limitations of enzymatic reactions as they relate to the organic media used and the concentration of water that must be present.

PROJECT HIGHLIGHTS FOR FY 1996

- *Directed Evolution of pNB Esterase*. The project team has increased the activity of an industrial enzyme (pNB esterase from Eli Lilly) by more than 150-fold, using random recombination (DNA shuffling). The sequences of a series of mutant enzymes along the evolutionary pathway have been determined, and biochemical characterization has been completed. This project has clearly demonstrated the power of directed evolution methods to create novel activities in natural enzymes and to extend their function to nonnatural environments. Eli Lilly has had a patent application filed on this enzyme and has exercised its option to license this enzyme for β-lactam production.
- *Evolution of Subtilisin as a Peptide Ligase.* Directed evolution methods have been successfully applied to the evolution of a peptide ligase from Subtilisin E. This year, mutants were identified that provide up to twice the conversion as the wild type enzyme and are also more stable. A collaborative research contract was completed with Recombinant Biocatalysis, Inc., which is now developing other industrial enzymes through the methods used in this project.
- A patent application was filed in January 1996. F. H. Arnold, "Improved para-Nitrobenzyl Esterase Enzymes by Directed Evolution," Ser. No. 08/589,892.
- Moore, J. C. and Arnold, F. H.. 1996. "Directed Evolution of a para-Nitrobenzyl Esterase for Aqueous-organic Solvents." *Nature Biotechnology*, **14**: 458-467. (This paper was the cover article.)
- You, L. and Arnold, F. H. 1996. "Directed Evolution of Subtilisin E in *Bacillus subtilis* to Enhance Total Activity in Aqueous Dimethylformamide." *Protein Engineering*, **9**: 77-83.

PARTICIPANTS/PARTNERS

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Flexible Chemical Processing of Polymeric Materials

BACKGROUND

A process for converting mixed polymer waste streams into valuable chemicals, saving energy, lowering production costs, and reducing the amount of waste going to landfills.

Waste textiles and recycled waste materials from automobiles, appliances, and furniture contain polymers (such as nylon-6, nylon-66, PET, and polyurethanes) that can be converted into valuable chemical feedstocks. However, processes that can only convert a single type of recycled material can face high costs for material collection and for transportation of the resulting feedstocks. Because these costs are the major contributors to process costs, processes are needed that can convert a variety of recycled materials.

This project will develop a thermochemical process that can convert a wide variety of recycled materials into valuable chemicals. A two stage process will be used: the first will use selective catalytic pyrolysis to recover chemicals such as caprolactam, hexamethylenediamine, and dimethyl-terephthalate; the second will convert the unreacted organic material into synthesis gas, which can be converted to a variety of chemicals of use to the chemical industry.

Because the process can address a wide variety of recycled materials, large regional processing plants can be developed, lowering material collection and transportation costs and thereby increasing the viability of recycling many materials.

ENERGY SAVINGS AND ENVIRONMENTAL BENEFITS

By the year 2020, the use of this technology will provide the following annual benefits:

- 265 trillion Btu of energy savings
- 1.75 million tons less waste going to landfills
- $1.46 million in production cost savings.

PROJECT HIGHLIGHTS FOR FY 1996

- Design and deployment of the Thermochemical User's Facility at the National Renewable Energy Laboratory was completed.
- A presentation on specialized capabilities was presented to industrial partners and trade associations for future evaluations of pilot scale chemical processing.
- Discussions were initiated with a large chemical company on potential collaboration in polymer recycling.

PARTICIPANTS/PARTNERS

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Inorganic Membrane Reactor Technology

BACKGROUND

Membrane reactor technology that separates hydrogen and oxygen efficiently, reducing energy consumption and waste generation in the petrochemical industry.

Many petrochemical processes are highly energy intensive while suffering poor conversion efficiency. For example, in producing propylene (a fundamental building block for common plastics and other petrochemical applications) by removing hydrogen from propane, the current conversion efficiency is only about 57%. These poor efficiencies, along with high energy consumption and related emissions, lead to economic and environmental impacts for many other processes.

This project develops membrane-based technology that will positively impact many large volume processes through a new reactor design. To demonstrate the utility of the new proposed technology, four processes have been chosen that are also attractive for possible future incorporation throughout the petrochemical industry: (1) production of methanol, (2) production of MTBE, (3) dehydrogenation of propane to produce propylene, and (4) dehydrogenation of ethylbenzene to produce styrene.

ENERGY SAVINGS AND ENVIRONMENTAL BENEFITS

By the year 2010, the use of this technology will provide the following annual benefits for the four identified processes:

- 130 trillion Btu of energy savings
- 0.3 million tons of volatile organic compound (VOC)/fugitive emissions avoided.

PROJECT HIGHLIGHTS FOR FY 1996

- The long-term stability of silica and palladium membranes in membrane reactor dehydrogenation processes was studied. Silica membranes demonstrated superior stability under dehydrogenation conditions, although further improvements in long-term stability are required prior to commercialization.
- In propane dehydrogenation, it was demonstrated that a membrane reactor could generate the same propylene yield as a conventional reactor that was twice as large. In constructing a new propylene production facility, reactor size can therefore be reduced, and capital investment costs lowered.
- For isobutane dehydrogenation, it was demonstrated that by using a membrane reactor operated at a reasonable flow rate, the thermodynamic limitations associated with operating at high pressure could be overcome to obtain a reasonable isobutylene yield. This result implies that, unlike conventional dehydrogenation reactors, membrane reactors can potentially be operated at elevated pressures, reducing refinery plant plumbing requirements, which can lower capital costs.
- Determined, through evaluating membrane reactor performance under a variety of operational conditions, improvement in the stability of dehydrogenation catalysts is required to take advantage of the potential performance gains offered by membrane reactors.
- Fabrication procedures for the preparation of a microporous metal/ceramic membrane were developed. During testing, the membrane demonstrated improved hydrogen permselectivity compared to molecular sieving porous silica membranes.

PARTICIPANTS/PARTNERS

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Inorganic/Polyphosphazene Membrane

BACKGROUND

A membrane that can be used in organic solvents and harsh environments, decreasing process costs and increasing flexibility.

Polymeric membranes have been used for many years for a variety of commercial separations processes, such as those used to upgrade natural gas, produce industrial gases, and desalinate seawater. Polymeric materials offer several advantages for these applications, including relatively low materials cost; the ease of forming a thin, defect-free film for either flat sheets or hollow fibers; and the ability to fabricate robust membrane modules. However, the use of polymeric materials has been restricted by their low resistance to organic solvents and limited thermal stability.

Under this project, OIT and the Idaho National Engineering Laboratory (INEL) have developed a new class of polymers for membrane separations that overcomes the limitations of traditional polymeric materials. Membranes made from these new polymers, known as polyphosphazenes, can be designed to have high solvent resistance and can operate in high temperatures and/or harsh environments. Polyphosphazene membranes have the ability to separate chlorinated hydrocarbons and other organics from water, and acid gases from other gases. In addition, the properties of polyphosphazene materials can be tailored to specific applications. Separation energy requirements can be reduced by about one-third using the new membrane-based process.

Currently, research is underway to 1) develop methods for coating the surfaces of multilumen porous ceramic tubes with a thin layer of polymer, and 2) develop and test new polymers and membranes.

ENERGY SAVINGS AND ENVIRONMENTAL BENEFITS

By the year 2010, the use of this technology (with 600 operating units) will provide the following annual benefits:

- 39 trillion Btu of energy savings
- 2.4 million tons of waste emissions avoided, including 80 tons of particulates, 100 tons of VOCs, 520 tons of SO_x, 2,700 tons of NO_x, and 2,354,000 tons of CO_2.

PROJECT HIGHLIGHTS FOR FY 1996

- A manually operated, pallet-sized, polymer-based pervaporation system was completed and will be tested using host site feed streams.
- Promising polyphosphazene membranes were developed to remove methyl chloride from water and to remove water from ethylene glycol.
- A patent application was filed relating to a method for coating porous ceramic substrates with thin polymer membranes.
- Peterson, E.S. "Industrial Opportunities for Recovery of Organic Chemicals." Invited paper presented to the U.S. EPA, National Risk Management Research Laboratory, Sustainable Technologies Division. November 18, 1996.
- Peterson, E.S., F.F. Stewart, M.L. Stone, C.J. Orme, and M.N. Tsang. "Molecular Separations Using Polyphosphazene Membranes." Presented at the American Institute of Chemical Engineers meeting. November 14, 1996.

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Levulinic Acid: New Derivatives

BACKGROUND

Chemical derivatives that save money, save energy, and reduce waste by using levulinic acid made from renewable resources as a chemical feedstock.

Each year, the U.S. pulp and paper industry produces millions of tons of paper sludge containing wastewater treatment materials that are also rich in carbohydrates. Because the heat value of this material is too low to justify burning it for cogeneration purposes, it is typically landfilled. However, recent R&D has suggested that a high-value chemical intermediate known as levulinic acid could be manufactured from this sludge using high temperature, dilute acid hydrolysis.

Levulinic acid has potential uses in the manufacture of numerous high-value chemical products and liquid fuels. However, its high cost inhibits large-scale use. This project seeks to improve and commercialize the conversion of biomass-based levulinic acid into commodity and specialty chemicals and to develop new uses for inexpensive levulinic acid. Three processes are being investigated: 1) the conversion of levulinic acid into new monomers and chemical intermediates; 2) an improved preparation of delta-amino-levulinic acid (5-ALA), a promising herbicide and pesticide; and 3) conversion of levulinic acid into methyltetra-hydrofuran (MTHF), a promising fuel extender.

ENERGY SAVINGS AND ENVIRONMENTAL BENEFITS

Use of levulinic acid derived from paper sludge could reduce the amount of waste going to landfills and displace some use of petroleum feedstocks. By the year 2010, this project will result in the following annual benefits:

- 102 trillion Btu of energy savings
- 9.3 million tons of waste reduced.

PROJECT HIGHLIGHTS FOR FY 1996

- Several approaches to developing a simplified process for producing 5-ALA were examined. A reagent was discovered that seems to effect the needed transformation, but not at the desired location. Further work will investigate the conditions necessary to optimize the reaction such that it will occur at the proper location in the molecule.
- Investigations were initiated to determine how production processes for MTHF might be optimized to increase their efficiency and to lower MTHF costs, which are otherwise prohibitively high.

PARTICIPANTS/PARTNERS

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Novel Waste Conversion Process for Recovery of Valuable Chlorosilanes

BACKGROUND

A process that saves energy and reduces the amount of waste that must be landfilled by recovering silicon and other valuable elements from the reactions used to produce chlorosilanes (the primary precursors of silicones).

New technologies are needed that would enable silicone producers to recycle wastes associated with the production of silicone. One such technology being developed will convert chlorosilane monomers, dimers, and heavier silicon-containing compounds into useful chemical intermediates.

The OIT is working with industry to convert silicone byproducts of limited value into methylchlorosilane intermediates that can be recycled through the silicone production process as a feedstock. Recycling saves energy by displacing raw materials used to produce silicone and by increasing chloride recycle efficiency. Another benefit is a reduction in the landfilling of direct process residue (DPR), one of the byproducts recovered in the new process. The recovery of DPR conserves the considerable embodied energy of the silicon contained within it.

ENERGY SAVINGS AND ENVIRONMENTAL BENEFITS

By the year 2010, the use of this technology could provide the following annual benefits:

- 521 trillion Btu of energy savings
- 148,000 tons of waste production avoided.

PROJECT HIGHLIGHTS FOR FY 1996

- A pilot scale test of the technology was authorized in Carrollton, KY, to start in March 1997. The plant will process about a half-ton per day of silicone wastes.

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Plastics, Fibers, and Solvents from Biosynthetically Derived Organic Acids

BACKGROUND

Production of chemical intermediates from corn-based feedstocks that conserves valuable petroleum resources, lowers costs, and avoids the generation of wastes.

Succinic acid is an intermediate in the chemical manufacture of commodity plastics (for use in automobiles and household items), fibers (for use in clothing), solvents (for paints and paint removers), and food additives. Currently, several hydrocarbon-based processes are used to make succinic acid. The acid can also be made biologically using corn syrup. This approach avoids the use of a petroleum feedstock; however, for every 100 million pounds of succinic acid produced through this route, 120 million pounds of the byproduct gypsum are generated, which must be sent to landfills. An environmentally favorable process is needed that does not generate undesirable byproducts.

The goals of this project are 1) to demonstrate the feasibility of producing succinic acid from cornstarch without producing gypsum waste, and 2) to demonstrate the economically competitive production of derivatives, such as 1,4-butanediol, from biologically-produced succinic acid. Research is also underway to incorporate more advanced processing technologies that will further reduce the cost of biologically-produced succinic acid and its value-added products. This effort includes expanding the viable products from the core succinic acid platform to a suite of chemicals that might include tetrahydrofuran, gamma butyrolactone, N-methyl pyrrolidinone, and polyesters.

ENERGY SAVINGS AND ENVIRONMENTAL BENEFITS

By the year 2010, the use of this technology will provide the following annual benefits:

- 20 trillion Btu of energy savings
- 0.7 million tons of waste production avoided.

PROJECT HIGHLIGHTS FOR FY 1996

- Applied CarboChemicals agreed to manufacture chemical feedstocks from renewable farm crops at a significantly lower cost than conventional petroleum-based methods. The new process produces succinic acid by fermenting glucose sugar from corn, then separates and purifies the acid and uses it as an intermediate to produce 1,4-butanediol, tetrahydrofuran, N-methyl pyrrolidinone, and other chemical feedstocks.

- Fermentation characteristics for a new strain of succinic acid-producing microorganism were determined at the laboratory scale.

- A patent application was submitted for a mutant E. Coli strain, AFT111, that exhibits increased succinic acid production. M. Donnelley and C. Millard, Argonne National Laboratory, ANL-IN-95-055.

- Millard, C.S., Y.-P. Chao, J.C. Liao, and M.L. Donnelley. 1996. "Enhanced Production of Succinic Acid by Overexpression of PEP Carboxylase in E. Coli." *Appl. Environ. Microb.* **62**: 1808-1810.

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Polyols from Sorbitol

BACKGROUND

Improvements in catalysis, separation, and processing in the production of polyols from sorbitol that save energy and avoid the use of petroleum feedstocks.

Currently, the oxidation process used to make polyol (poly alcohol) chemicals from petroleum feedstocks is inherently energy inefficient and perpetuates this country's reliance on imported oil. As a replacement for petroleum feedstocks, sorbitol may be produced from corn starch-based glucose and further processed into a suite of valuable chemicals known as polyols.

The ability to selectively favor the production of one polyol product or another is important in making this process economical. In this case, sorbitol is the chemical intermediate, and the work by Pacific Northwest National Laboratory (PNNL) and International Polyol Chemicals, Inc. is designed to add value to this inexpensive feedstock such that the overall process is suitable for scale-up into the market.

ENERGY SAVINGS AND ENVIRONMENTAL BENEFITS

By the year 2010, the use of this technology will provide the following annual benefits:

- 16.6 trillion Btu of energy savings.

PROJECT HIGHLIGHTS FOR FY 1996

Batch and continuous-flow reactor tests were used to evaluate the range of optimum production of glycerol from sorbitol using improved nickel metal catalysts. The industrial partner has proposed using the developments in a small plant at a major corn processor's facility.

A patent application has been filed on the stabilized nickel metal catalysts for use in this technology and other aqueous phase hydrogenation processing systems.

PARTICIPANTS/PARTNERS

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Precursors for Specialty Plastics from Renewable Feedstocks

BACKGROUND

Precursors for specialty plastics from renewable feedstocks that may be used to replace petrochemical precursors, reducing both energy use and environmental impacts.

The goal of this project is to develop a biocatalyst and a bioprocess based on fermentation that will reduce the manufacturing costs of a key monomer used to produce certain types of thermoplastics. Engineering thermoplastics are used worldwide in applications that range from compact disks to automotive and airplane parts, to computer and appliance housings, to bullet-resistant glazing. Within the engineering thermoplastics market, the high-performance materials offer many attractive characteristics, including excellent processability, outstanding strength, superior chemical resistance, the ability to withstand extreme heat, and recyclability. However, the use of these high-performance products has been relatively limited because of their high cost. These materials might find wider use if the manufacturing costs could be reduced. A key to meeting this challenge is to reduce the costs of thermoplastic chemical building blocks.

The technical challenge is considerable because the technology must be driven by the process economics in addition to the development of the biocatalyst and bioprocess. This project will lead to the process design and economic data necessary to determine the commercialization potential of the technology. The new biocatalysis system could lead to new markets for renewable feedstocks (such as domestic corn), could reduce dependence on petroleum imports, and could avoid generating the waste streams associated with the petrochemical production process. The availability of lower-cost, high performance engineering thermoplastics also may improve the performance of parts and reduce manufacturing costs for many applications, leading to their use in much broader markets.

ENERGY SAVINGS AND ENVIRONMENTAL BENEFITS

By the year 2010, the use of this technology will provide the following annual benefits:

- 3.1 trillion Btu of energy savings.

PROJECT HIGHLIGHTS FOR FY 1996

- General Electric Company and Lockheed Martin Idaho Technologies Company, the prime contractor at the Idaho National Engineering Laboratory (INEL), are working together to develop a biocatalyst and a bioprocess that will reduce the production cost of a key monomer. The feedstock for this fermentation process will be a renewable feedstock such as corn, one of the United States' most plentiful agricultural products. The overall process is being developed and optimized to minimize raw materials costs and maximize monomer recovery and purification.

PARTICIPANTS/PARTNERS

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Process for Producing Phenolics from Wood Waste

BACKGROUND

A process for producing phenolics from biomass feedstocks that is 33% to 50% less costly than deriving phenol from petroleum products, saves energy, avoids the use of non-renewable petroleum feedstocks, and reduces biomass wastes.

The wood composites that are often used in place of solid wood in furniture and other products are manufactured with adhesives made from phenol formaldehyde (PF) resins. These resins are also used for production of crosslinked plastics (Bakelite or novolacs). Production of PF resins requires more than one billion pounds of relatively expensive petroleum-based phenol each year. Because these resins do not require high-purity phenol, it is feasible to use low-cost phenolics derived from waste biomass to replace a large portion of the petroleum feedstock requirement for resin production.

OIT and industry have been sharing the cost of developing low-cost, high-performance adhesives specifically tailored for composite wood products. Scientists at the National Renewable Energy Laboratory (NREL) have developed a process that uses ablative fast pyrolysis and solvent extraction to convert waste biomass or lignin into a phenol-rich oil that can be formulated directly into PF resins or combined with petroleum-derived phenol to produce PF resins that meet industrial standards. Depending on the cost of the biomass feedstock and the size of the pyrolysis plant, the cost of the phenol replacement is only one-half to two-thirds the cost of phenol derived from petroleum products. The process is energy self-sufficient, using some of the non-phenolic biomass material as fuel for the pyrolysis reactor.

ENERGY SAVINGS AND ENVIRONMENTAL BENEFITS

By the year 2010, the use of this technology will provide the following annual benefits:

- 8 trillion Btu of energy savings
- 618,000 tons of biomass waste reduced.

PROJECT HIGHLIGHTS FOR FY 1996

- A synthetic approach was developed for converting crude oils or fractions to higher value chemicals.

- Process development was completed and the performance of the chemicals produced using this route was verified in specific applications.

- A separate project was developed with Mineral Technologies, Inc. (MTI) to use chemicals produced through the processes developed in this project. MTI will use the chemicals for stabilization of paper brightness.

- An investigation was initiated into using pyrolysis to convert phenolic-rich plastics to high value industrial chemicals for use in thermoset plastic production.

PARTICIPANTS/PARTNERS

The development of this technology is supported by the Pyrolysis Materials Research Consortium, which includes five industrial members: AlliedSignal, Aristech Chemical Company, Plastics Engineering Company, Interchem, and MRI Ventures, Inc.

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Processes for Recovery of Automobile Shredder Residue (ASR) and Recycled Materials from Appliances

BACKGROUND

Mechanical/chemical processes to recycle plastics and other materials from shredded automobiles and appliances that save energy, save natural resources, and reduce the amount of auto waste going to landfills by 14%.

Each year, landfill costs and liability issues related to scrap and waste from discarded automobiles and appliances increase. Yet at the same time about 5 million tons of automobile recycling residue are sent to landfills each year and less than 50% of the almost 3 million tons of discarded appliances are recycled. Moreover, the scrap value of discarded appliances has decreased as the use of plastics in appliance manufacture has increased.

The recycling process for these goods currently consists of shredding, recovery of metals and other economically valuable materials, and disposal of residue. In this project, improved separation technologies are being developed that will allow the economic recycling of polyurethane foam, thermoplastics, and iron oxides from ASR and the recovery of ABS/HIPS plastics from obsolete appliances.

ENERGY SAVINGS AND ENVIRONMENTAL BENEFITS

By the year 2010, the use of these technologies will provide the following annual benefits:

- 97.4 trillion Btu of energy saved
- 11.7 million tons of waste reduction
- 9 million tons of CO_2 emissions avoided.

PROJECT HIGHLIGHTS FOR FY 1996

Auto Shredder Residue

- A batch scale field demonstration recovered 2,000 pounds of polyurethane foam.
- A process for continuous polyurethane foam recovery and cleaning was designed and constructed.
- A laboratory-scale project proved the feasibility of recovering high-purity polycarbonate/ABS plastic alloy from disassembled auto parts.

Appliances

- More than 500 pounds of high purity ABS/High Impact Polystyrene plastics were recovered in large scale separation tests.
- Appliance Recycling Centers of America agreed to operate a plastics separation pilot plant in Minneapolis.

Publications

Jody, B.J., E.J. Daniels, and J.A. Pomykala, Jr. February 1996. "Progress in Recycling of Automobile Shredder Residue." Proc. Extraction and Processing Division, the TMS Annual Meeting, Anaheim, California.

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Karvelas, D.E., B.J. Jody, B. Arman, J.A. Pomykala, Jr., and E.J. Daniels. February 1996. "Recovery and Separation of High Value Plastics from Discarded Household Appliances." Proc. Extraction and Processing Division, the TMS Annual Meeting, Anaheim, California.

PARTICIPANTS/PARTNERS

Alter Trading Corporation, Appliance Recycling Centers of America, Vehicle Recycling Partnership (Ford, GM, and Chrysler), American Plastics Council, Woodbridge Group, Institute of Scrap Recycling Industries, Independent Center, David Joseph Company, and GE Specialty Chemicals.

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Production of Lactic Acid from Renewable Resources

BACKGROUND

Production of lactic acid that uses processes based on the fermentation of renewable resources (such as cellulosic waste) to produce biodegradable polylactic acid (PLA) as a replacement for petroleum-derived plastics.

About 60 million pounds of plastic goods are generated every year, posing a significant disposal problem. These plastics are produced almost entirely from petroleum-derived raw materials. The use of a biodegradable polymer such as polylactic acid (PLA) in place of existing polymers in plastics would alleviate the disposal burden. Moreover, producing the PLA from renewable resources would reduce the use of fossil fuels.

Lactic acid is an important chemical with a tremendous potential for future growth as a precursor for biodegradable PLA production. In order to make PLA economically viable and facilitate the penetration of existing polymer markets, an inexpensive source of lactic acid is crucial. the production of lactic acid via fermentation of a renewable resource, in particular, a cellulosic waste product, would not only replace fossil fuels with renewable resources, but would also efficiently utilize a waste product that would otherwise be a disposal problem. This project will significantly reduce lactic acid production costs in a commercial-scale process.

ENERGY SAVINGS AND ENVIRONMENTAL BENEFITS

By the year 2010, the use of this technology will provide the following annual benefits:

- 110 trillion Btu of energy savings
- 8.2 million tons of waste reduction
- 8.9 million tons of CO_2 emissions avoided.

PARTICIPANTS/PARTNERS

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Rational Enhancement of Enzyme Performance in Organic Solvents

BACKGROUND

Rational enhancement of enzyme performance in organic solvents that may be applied to processes of industrial importance.

Rigid protein configurations in enzymes retain the conformation (imprint) induced by the original ligand/stability factor. The result of this molecular memory is an enzyme with altered catalytic characteristics or a new binding site, which may be able to perform new chemical reactions.

This project will elucidate the mechanisms of enzyme stability in organic solvents and apply the knowledge to processes of industrial importance. The project will also investigate gas-phase biocatalysis and the phenomenon of "molecular memory" of enzymes. A better understanding of enzyme operations and performance in nonaqueous media will result. Work with AlliedSignal is focused on the development of optimum parameters for enzyme esterification reactions in nonaqueous media.

PROJECT HIGHLIGHTS FOR FY 1996

- The project team has discovered that the enantioselectivity of enzymes, as well as its temperature dependence, in organic solvents (in contrast to water) is markedly affected by the method of enzyme preparation.

- The main factors responsible for the drastically lower enzymatic activity in anhydrous solvents compared with water have been elucidated.

- A new methodology (Fourier-transform infrared, FTIR, spectroscopy) has been developed and validated to quantify the secondary structure of enzymes suspended in organic solvents, thus allowing heretofore impossible structure-activity correlations.

- A patent application was filed in the first quarter of 1996. A.M. Klibanov, K. Lewis, A.A. Ferrante, C.L. Coyle, G. Zystra, M.S.P. Logan, and M.L. Grossman, "Solvent-Resistant Microorganisms."

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Scrap Tire Recycling

BACKGROUND

Recycling of scrap tires through the development of a new surface treatment technology for finely ground tire rubber that allows it to be used in the manufacture of high value composites, thereby replacing petroleum-derived polymers.

Of the total number of scrap tires generated each year in the United States, over 50% are used as fuel competing with or partially replacing lump coal, with another 20% finding various other uses. The remaining 30%, or 70 million scrap tires, go to stockpiles each year. Currently, stockpiles contain an estimated 850 million scrap tires, representing 17 billion pounds of rubber.

This project will develop new surface treatment technology for incorporating finely ground tire rubber into high value composite materials.

ENERGY SAVINGS AND ENVIRONMENTAL BENEFITS

The petroleum-derived polymers that are displaced by the scrap tire crumb rubber have an embodied energy of 50,000 Btu per pound. The fuel value of the rubber is only 18,000 Btu per pound. This results in net energy savings whenever the scrap rubber can be used in these higher value products rather than used as fuel. The energy needed to convert the scrap rubber into useful crumb rubber is very small.

PROJECT HIGHLIGHTS FOR FY 1996

- Surface-modified rubber particles have been demonstrated to increase the impact resistance and toughness of several types of coatings and paints, including epoxies, polyurethane, and latex systems. Several improvements were developed for the process of manufacturing surface-modified rubber particles. These improvements include a method for removing fibers from tire cord in rubber, a technique for de-agglomeration of rubber particles, and a process for

reducing the moisture level in treated rubber. These process improvements reduce costs and increase the quality of surface-modified rubber, expanding the potential applications.

- Issued Patent Number 5,506,283, "Higher Modulus Rubber Compositions Incorporating Particulate Rubber," on April 9, 1996.

- Bauman, B.D. "Surface Modified Rubber Particles for Polyurethanes." In *Handbook of Additives*. To be published by Chapman and Hall, London.

- Bauman, B.D. "High Value Scrap Tire Recycle." Presented at the Clemson University Tire Industry Conference, Hilton Head, South Carolina, March 7, 1996.

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Selective Surface Flow (SSF™) Membranes for Waste Hydrogen Recovery

BACKGROUND

Membranes for waste hydrogen recovery that recover hydrogen from waste streams for use as a feedstock, thereby reducing NO_x and CO_2 production.

The U.S. petroleum and chemical industries produce very large volumes of hydrogen-containing waste gas streams (about 800 million SCFD) at low hydrogen concentrations (20-50%) and at low pressures (20-150 psig). The hydrogen from these streams is not economically recoverable by existing technologies and hence is either flared or used as fuel. There is an increasing demand for hydrogen in refineries because of Clean Air Act regulations. Thus, it would be useful to recover the hydrogen for its chemical value. Also, the use of hydrogen as fuel in such operations results in decreased NO_x production and CO_2 emissions.

Rather than separating hydrogen by molecular sieving, solution-diffusion, or Knudsen separation, the Selective Surface Flow (SSF™) technology separates by selective adsorption and surface diffusion through the nanopores of the membrane. This separation mechanism allows (1) the recovery of hydrogen on the feed side at feed pressure, (2) high separation selectivity because of selective adsorption and surface diffusion and pore blockage, (3) separation capability at low pressures, and (4) high flux, because of surface flow, resulting in low membrane area for separation. When coupled with a conventional hydrogen purification process (pressure swing adsorption), the membrane produces a high purity hydrogen stream.

ENERGY SAVINGS AND ENVIRONMENTAL BENEFITS

By the year 2010, the use of this technology will provide the following annual benefits:

- 16.6 trillion Btu of energy savings
- 382 tons of NO_x emissions avoided
- 890,000 tons of CO_2 emissions avoided.

PROJECT HIGHLIGHTS FOR FY 1996

- Bench scale research results were applied to the construction and operation of a 1 ft^2 membrane unit at the Air Products and Chemicals, Inc. (APCI) Hydrogen Facility at the Tosco Oil Refinery.
- A 1 ft^2 membrane system was demonstrated that was subsequently scaled up to a 1000 ft^2 semi-commercial membrane system being demonstrated at the APCI hydrogen facility in New Orleans, LA.
- Completed demonstrations have encouraged APCI to transfer the membrane technology focus from its corporate R&D to its business unit for future marketing, commercialization, and sales.

PARTICIPANTS/PARTNERS

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Separations by Reversible Chemical Association

BACKGROUND

Use of reversible chemical association to separate polar organic compounds from dilute aqueous solutions, thereby reducing energy requirements and waste generation compared with conventional separations.

The currently available options for separating polar organic compounds from dilute aqueous solutions — distillation, evaporation, and solvent extraction — are energy intensive. An alternative separation method uses complexing agents, which may be combined with polar organic compounds as a means of separation from dilute aqueous solutions. The complexation process is then reversed to regenerate the organic compounds.

This project is developing processes that will produce separations more energy efficiently than the currently available options. Polar organic solutes of interest include oxygenated compounds produced by fermentation, such as carboxylic acids, alcohols, and amino acids. The general objectives of the project include measurement of phase equilibria and the rates at which equilibria are established; establishment of guidelines for the selection of complexation agents; development of suitable methods of process integration (into other unit operations); and definition of the most promising applications of the separation method.

ENERGY SAVINGS AND ENVIRONMENTAL BENEFITS

The approaches being developed can substantially reduce the energy requirements of, and minimize the wastes generated by, conventional chemical separations in industry.

PROJECT HIGHLIGHTS FOR FY 1996

- *Recovery of Carboxylic Acids — Regeneration of Adsorbents*. Studies continued of methods for regenerating basic, amine-functionality polymeric sorbents, which are capable of recovering carboxylic acids from aqueous solutions above known hydrogen ion concentrations (pH) of the carboxylic acid. A solution of TMA in dry methyl isobutyl ketone (MiBK) provides a high degree of recovery of lactic acid from Dowex MWA-1. Thus leaching with a non-aqueous TMA/solvent mixture affords a means for recovery of lactic acid from basic resins, such as Dowex.
- *Recovery of Carboxylic Acids — Multi-Acid Equilibria*. Equilibria for simultaneous sorption of mixtures of carboxylic acids onto Dowex MWA-1 were measured. Separation of lactic and succinic acids by preferential sorption of succinic acid onto Dowex MWA-1 is possible at pH near 4, and separation of formic and acetic acids through preferential sorption of formic acid is possible at pH below 5. These results are directly relevant to current industrial needs.
- *Adsorption of Phenols onto Activated Carbons*. Adsorbed phenols are incompletely regenerable from activated carbons, because the carbon surface catalyses oxidative coupling of phenols. The results of experiments demonstrated that increasing surface acidity may reduce oxidative coupling by enhancing competitive sorption of water.
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- Dai, Y. and C.J. King. 1996. "Selectivity Between Lactic Acid and Glucose during Recovery of Lactic Acid with Basic Extractants and Polymeric Sorbents." *Ind. Eng. Chem. Research*. **35**: 1215-1224.

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Theory of Biocatalysis-Electron Transfer Reactions

BACKGROUND

A theory of biocatalysis-electron transfer reactions developed through computer-aided design methodologies for enzyme biocatalysts with tailored catalytic rates, applied to develop protein conversion systems.

Enzymes in biological systems speed up the rate of chemical reaction, acting as catalysts. A better understanding of the structure of enzymes may be applied to develop new biological catalysts. There are applications to a number of industries concerned with biocatalysis, such as DNA diagnostics, biosensors, and nonlinear optics.

This project will perform computer-aided design of enzyme biocatalysts with tailored catalytic rates. The focus of this project is on electron transfer enzymes, a major class of biological enzymes. The theory of protein electron tunneling pathway has been developed and implemented as computer models that connect enzyme electronic structures and their reaction rates.

Specific project objectives include: (1) development of algorithms to map the key residues in proteins between electron transfer sites that mediate electronic coupling and allow electron transfer reaction to proceed with great speed and specificity; (2) identification of "hot" and "cold" spots with respect to electron transfer in native and modified proteins; (3) development of an understanding of primary, secondary, tertiary, and quaternary structural effects on electron transfer rates; and (4) use of knowledge gained to stabilize energetic charge separated states and to enable the development of semisynthetic/modified protein energy conversion systems.

PROJECT HIGHLIGHTS FOR FY 1996

- Electron donor-acceptor interactions in DNA were computed using both workstation and supercomputer technology.
- Secondary structure effects on protein transfer were computed.
- New methods were developed to dissect donor-acceptor interactions in proteins into multi-pathways components.
- A working model for two-electron transfer reactions was developed that is capable of distinguishing between stepwise and concerted mechanisms.
- Approximately 200 copies of the search software have been issued to users in industry and academia.

PARTICIPANTS/PARTNERS

The University of Pittsburgh, Cray Research, the National Science Foundation (through a Young Investigator Award), the DuPont Company, Nanogen, and the Beckman Institute.

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Waste Carpet Recycling

BACKGROUND

Recycling of waste carpet into useful chemicals, saving energy, reducing the amount of waste carpet going to landfills, and reducing the generation of ammonium sulfate and other wastes.

Approximately 3.5 billion pounds of waste carpet are discarded each year, contributing to landfill saturation. The overall goal of this project is to develop a novel process to recycle nylon carpets, including the backing materials.

Approximately 30% of the carpets sold in the U.S. are made from nylon 6. This project will develop a laboratory-size unit for continuously extracting nylon 6 and non-nylon 6 hydrolytic degradation products from whole or partially separated nylon 6 carpet. Following this, a continuously operated depolymerization tubular reactor will be developed and built to reduce the nylon 6 to the caprolactam monomer. The high purity caprolactam that is separated from this mixture can be used to make new nylon 6 fibers. The non-nylon 6 components (such as styrene-butadiene-styrene, styrene-butadiene-rubber, and calcium carbonate) that will also be extracted will be used as modifiers for industrial tar products, particularly roofing membranes.

Manufacture of new caprolactam is energy intensive and creates large amounts of ammonium sulfate and other waste products. This waste generation will be eliminated by the reclamation technology being developed under this project.

ENERGY SAVINGS AND ENVIRONMENTAL BENEFITS

By the year 2010, the use of this technology could provide the following annual benefits:

- 19.6 trillion Btu of energy savings (for four, 100 million lb/yr caprolactam plants)
- 8 to 25 million pounds of chemical effluent waste reduced
- Over 10 billion pounds of municipal solid waste reduced.

PROJECT HIGHLIGHTS FOR FY 1996

- A continuous 24-hour operation test was completed for conversion of nylon 6 to caprolactam, demonstrating high yield and reproducibility.
- Based on tests with a pilot scale unit, an evaluation of process economics, feedstock preparation, and product purification was completed.
- The potential for using pyrolysis processes obtaining chemicals from different industrial and post-consumer polymer wastes was evaluated.

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Advanced Membrane Device

BACKGROUND

Active transport membrane processes differ from other membrane separation processes because they involve specific chemical reactions rather than filtration or reliance on differences in solubility among a mixture's compounds. An "active transport" material is embedded into a membrane, where it selectively extracts a component of the mixture being fed into the system and transports it through the membrane for release on the other side. The technology is more energy efficient than current gas absorption and liquid extraction technology. The specific focus of this research is acid gas separation from methane as part of natural gas production.

The project team had difficulty achieving the needed permeance and selectivity for the hollow-fiber membranes that were being tested. The team also had difficulty removing water using the active transport membranes. In the course of trying different materials, the team tested a particular polymeric material and achieved good results. The team is now using this polymeric material as the coating material in place of the active transport material, but the objective of acid gas separation from methane remains unchanged.

ENERGY SAVINGS AND ENVIRONMENTAL BENEFITS

By the year 2010, the use of this technology (with 1,560 units operating) will provide the following annual benefits:

- 39 billion Btu of energy savings
- An increased amount of usable gas in gas reserves
- Lower greenhouse gas emissions due to reduced natural gas losses, flaring, and/or venting.

PROJECT HIGHLIGHTS FOR FY 1996

- The project team evaluated and set polymer membrane performance goals for permeance/ selectivity, cost, and hollow fiber fabrication.

- Two polymer groups (Active Membrane Devices - AMDs) with acceptable properties for scale-up and fabrication were identified.

- A polymer scale-up partner was identified and AMD synthesis at the 7 lb batch size was demonstrated.

- Pilot plot spining of AMDs hollow fiber membrane was demonstrated. Laboratory test loops of membrane fiber displayed the intrinsic permeance/selectivity of AMD dense film and exhibited acceptable tensile strengths.

PARTICIPANTS/PARTNERS

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Applications for Diesel Valve Guides (CFCCs)

BACKGROUND

The diesel engines currently used in some industrial and agricultural applications present a significant opportunity for energy savings and emissions reductions using continuous fiber ceramic composites (CFCCs). The cast iron valve guides used in current engines cannot operate at temperatures above 300ºC because the cast iron has insufficient strength, resulting in valve deformation and eventual failure. These valves also require regular lubrication with commercial petroleum-based lubricants to maintain proper operation. Even if a valve could operate at higher temperatures, available lubricants develop deposits that can cause the valve to stick or wear excessively. However, the energy efficiency of the diesel engine increases with elevated operating temperature.

As part of the OIT CFCC program, this project is examining a self-lubricating, CFCC diesel engine valve guide using a continuous carbon fiber-reinforced silicon nitride, which will be fabricated into components by one of several novel processing methods under consideration. The valve guide will provide the required friction and wear properties along with the structural integrity to operate under extreme temperature conditions.

ENERGY SAVINGS AND ENVIRONMENTAL BENEFITS

By the year 2010, the CFCC program (as a whole) will provide the following annual benefits:

- 600 trillion Btu of energy savings
- 980,000 tons of NO_x emissions avoided
- 119 million tons of CO_2 emissions avoided
- CFCC component sales of $850 million, adding over 8,000 industrial sector jobs.

PROJECT HIGHLIGHTS FOR FY 1996

- New net shape fabrication improvements were developed that result in reduced machining costs. These improvements minimize warpage of CFCC tube stock, increase the yield of CFCC tube stock with minimized cracking, and reduce the ratio of inside diameter/outside diameter machining stock by more than 20%.
- A 2-piece concept for a valve guide was developed that reduces cost. This concept has the potential for high speed, automated near-net-shape forming; requires a lower quantity of CFCC material per valve guide; and has the potential to reduce machining time by half.
- Durability was tested using a CFCC valve guide in a simulated diesel engine environment for 200 hours. Surface wear as measured for the valve guide was substantially less than the standard cast iron valve guide.

PARTICIPANTS/PARTNERS

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Atmospheric Recovery and Regeneration in Heat-Treating Operations

BACKGROUND

Heat-treating and similar high-temperature furnace operations typically maintain a reducing gas "atmosphere" to process iron and steel products. A major furnace operation is "carburizing" - heat treating of steel parts in the presence of gaseous carbon monoxide to produce hard, wear-resistant surfaces. An estimated 4500 U.S. manufacturing plants use carburizing furnaces, most of which have atmospheres produced by partially combusting natural gas and air in a catalytic chamber. Typically, the waste atmosphere gas is directly discharged into the environment through gas flares without additional pollution controls. This practice introduces high concentrations and large amounts of carbon monoxide into the environment and wastes the embodied energy of the carburizing atmosphere.

ENERGY SAVINGS AND ENVIRONMENTAL BENEFITS

By the year 2010, the use of this technology will provide the following annual benefits:

- 2.8 trillion Btu of energy savings
- 24,000 tons of toxic gas emissions avoided
- 66,000 tons of process CO_2 emissions avoided.

PROJECT HIGHLIGHTS FOR FY 1996

- This project has developed a new process that will reduce more than 90 percent of the furnace atmosphere gas discharged from furnaces. Dana Corporation's Spicer Off-Highway Axle Division plant in Plymouth, MN will demonstrate the carburizing atmospheric recovery and regeneration technology.

- The design of the recycling apparatus was completed, and all of the equipment needed for the commercial demonstration unit was ordered. Preliminary tests on the membranes have shown favorable results.

PARTICIPANTS/PARTNERS

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Bioconversion of Molasses By-Product to Organic Phytochelates

BACKGROUND

Environmental problems associated with overuse of nitrogen fertilizers have been well documented. Consequently, limitations on fertilizer use have been imposed in several countries. At the same time, fertilization of forest biomass has been identified as a cost-efficient option for mitigating global warming. The increased use of fertilizers to address problems of food availability and global warming will lead to increased nitrogen pollution of the environment.

A major goal of this project is to develop a method to increase fertilizer efficiency. Bioconversion of low value by-products from sugarcane will be used as a source of organic acids that can add value to fertilizers by acting as chelating agents (phytochelates) and increasing the availability of metal nutrients to plant tissue.

The project will 1) develop a cost-effective chromatographic separation of sucrose from cane molasses; 2) produce and recover succinic and lactic acids from the raffinate stream; and 3) test the organic acids as phytochelates in controlled laboratory studies, greenhouse studies, and field trials.

ENERGY SAVINGS AND ENVIRONMENTAL BENEFITS

By the year 2010, the use of this technology will provide the following annual benefits:

- 5.5 trillion Btu of energy savings
- 3.0 million tons of waste water
- 0.2 million tons of CO_2 emissions captured.

PROJECT HIGHLIGHTS FOR FY 1996

- The head weight of fieldsport cabbage, tested at the Michigan State Horticulture Teaching & Research Center, increased by 109% to 111% when selected raffinate-based biostimulants were applied to the soil at different stages of the plant growth cycle. In biostimulant tests at Michigan State University, bell pepper yield increased by as much as 156% by weight.

PARTICIPANTS/PARTNERS

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Climate Wise

BACKGROUND

The Climate Wise Program operates as a partnership between U.S. industry and the Federal Government and focuses on the highest energy-consuming processes and technologies currently used by OIT's Vision Industries. The Program encourages these industries to take advantage of the economic and environmental benefits associated with the adoption of advanced energy-efficient technologies that prevent pollution and reduce overall greenhouse gas emissions. In cooperation with Climate Wise at the Environmental Protection Agency (EPA), industrial partners are expected to set and achieve meaningful emission reduction goals; undertake specific actions to address energy, source, process, materials, and behavioral problems; and report the reductions through the Voluntary Greenhouse Gas Reduction Reporting System established under 1605(b) of the Energy Policy Act of 1992. In return for adopting new management practices and technology-based solutions, DOE and EPA will recognize each Climate Wise partner for improving industrial productivity and performance and serving as a steward of the environment. The program also offers workshops and provides information and assistance on technical subjects and business practices that will enable industry to maximize its contribution to a cleaner environment.

PROJECT HIGHLIGHTS FOR FY 1996

- There are over 200 industrial partners nationwide, covering almost all of the U.S. major manufacturing Standard Industrial Classification (SIC) codes. This includes participation by U.S. industry's highest energy consumers, such as Fortune 500 partners representing the forest products, chemical, petroleum refining, and steel industries.

PARTICIPANTS/PARTNERS

- 16 state government initiatives in New York, California, Maine, Utah, Iowa, Maryland, Connecticut, Tennessee, Nebraska, Alabama, Colorado, North Carolina, Ohio, Wisconsin, Oregon, and Pennsylvania.
- 6 city/county initiatives in Austin, TX; Berkeley, CA; Metropolitan Dade County, FL; City and County of Denver, CO; Portland, OR; and Tucson, AZ.
- The American Institute of Pollution Prevention.
- The Electric Power Research Institute.
- The Business for Social Responsibility Educational Fund.

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Design, Characterization, and Testing of Multimetallic Catalysts

BACKGROUND

The use of supported bimetallic catalysts in industry is extensive in spite of the general lack of fundamental understanding of how the small metal particles interact with the reacting species. The present activity focuses on one very important application, pollution control catalysts, with the intent of generating the scientific basis needed to design the next generation of catalysts in an efficient manner.

This project seeks to develop and implement computational methods of modeling small bimetallic particles composed of on the order of 100 to 1,000 atoms; to predict morphology and surface properties as a function of composition, reactive environment, and support material using these methods; and to test and validate the predictions experimentally using traditional techniques as well as unique, solid state NMR studies of metals and adsorbates. The major challenge for this program is the application of the modeling and experimental technique developed at the Ames Laboratory to more complex catalysts.

PROJECT HIGHLIGHTS FOR FY 1996

- The heats of adsorption of hydrogen (H) on rhodium (Rh), nickel (Ni), ruthenium (Ru), and platinum (Pt) monometallic catalysts, as well as a variety of bimetallic and promoted catalysts, have been measured for various H coverages, pressures, temperatures, and metal dispersions using microcalorimetry. These data can be used as input to the simulation procedures described below.

- The DeCAL (Design of Catalysts at Ames Lab) software has been made easy to use by the addition of a graphical user interface for both Silicon Graphics workstations using the UNIX operating system and personal computers using the Windows NT operating system.

- The DeCAL software has incorporated adsorbates, with explicit parameters determined and validated for H-Rh and H-Pt via comparison to NMR experiments on H/Rh/Pt supported clusters.

- A collaborative effort with Exxon researchers (who perform X-ray diffraction experiments) has yielded the structures of Cu_xPd_{1-x} clusters with diameters of 40-60 Å and composition range, x=0.1–0.7.

- Wetzel, T., L. Zhu, and A.E. DePristo. "CEMBOS software program for simulation of structure and microstructure of clean and adsorbate covered bimetallic clusters." Initial Program released to DuPont, Exxon, and GM on 9/3/96.

- Narayan, R.L., N. Savargaonkar, M. Pruski, and T. S. King. 1996. "Hydrogen Chemisorption and Mobility on Ru/SiO_2, K/Ru/ Ru/SiO_2, and Ru-Ag/ Ru/SiO_2." *Studies in Surface Science and Catalysis*, **101**: 921.

- Savargaonkar, N., B.C. Khanra, M. Pruski, and T.S. King. 1996. "Influence of Hydrogen Chemisorption on the Surface Composition of $Pt\text{-}Rh/Al_2O_3$ Catalysis." *J. Catal.*, **162**: 277 (1996)

PARTICIPANTS/PARTNERS

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Development of Asphalts and Pavements Using Recycled Tire Rubber

BACKGROUND

The efficient and environmentally sound disposal of used tires is an increasingly important need. Approximately 285 million tires are discarded each year, with only 35% being recycled. In an effort to alleviate this problem, the U.S. Government has mandated that tire-rubber be used in future asphalt pavement construction. The use of scrap tire-rubber, also known as crumb rubber modifier (CRM), as a modifier of asphalt cement is not new to the paving industry of the United States. However, the use of CRM in hot mix asphalt concrete has only met with sporadic success. As a result, state highway engineers are required to build CRM asphalt pavements without the needed experience, design parameters, specifications, and construction guidelines.

This project is pursuing several innovations that will provide the materials and knowledge needed for successful construction of CRM asphalt pavements and for improved performance of the pavements once in place. The first innovation is determining the optimal asphalt-rubber variables, such as the composition of the asphalt-rubber mixture, the rubber particle size, the rubber type, and the manufacturing process for the asphalt-rubber mixture. The second involves modifying the asphalt through supercritical fractionation (because the composition of the asphalt-rubber is determined not only by the amount of rubber in the asphalt, but also by the chemical nature of the asphalt itself). Through supercritical fractionation, the optimum asphalt chemical composition for superior asphalt rubber binders can be obtained. Additionally, supercritical fractionation will produce superior asphalt-rubber recycling agents. Finally, an advanced road aging simulation procedure developed at Texas A&M University will be used to determine the aging characteristics of asphalt-rubber blends and asphalt-rubber/recycling agent blends.

ENERGY SAVINGS AND ENVIRONMENTAL BENEFITS

By the year 2010, the use of this technology should provide the following annual benefits:

- 67 trillion Btu of energy savings
- 8.2 million tons of waste reduction.

Technology benefits include less landfill material, less virgin aggregate, and liquid asphalt. In addition, road life should improve, leading to fewer road replacements.

PROJECT HIGHLIGHTS FOR FY 1996

- Crumb rubber, dissolved in asphalt by high temperature, high sheer blending, and mild oxidation, produced rubberized-asphalts with improved properties.
- Rubberized-asphalts demonstrated improved asphalt-to-aggregate adhesion.
- It was demonstrated that lower cost, larger rubber particles can be used.

PARTICIPANTS/PARTNERS

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Development of Superior Asphalt Recycling Agents

BACKGROUND

About 27 million tons of asphalt and nearly twenty times as much aggregate are consumed each year to build and maintain over two million miles of roads in this country. Some recycling is being done, but results do not always produce asphalt that is as durable as new asphalt. The only significant impediment to wider adaptation of this recycle technology is the lack of adequate specifications for high-quality recycling agents capable of rejuvenating much or all of the hard, older asphalt material into a ductile, long-lasting material with "new material" properties.

In this project, various aged asphalts will be produced, characterized, and tested with candidate recycling agents as an initial screening for appropriate combinations of recycling agent and aged asphalt. Processing conditions and procedures for commercial production of recycling agents and for recycle blending will be developed.

ENERGY SAVINGS AND ENVIRONMENTAL BENEFITS

By the year 2010, the use of this technology should provide the following annual benefits:

- 180 trillion Btu of energy savings
- 90 million tons of aggregate rock waste reduced.

Technology benefits include less landfill material, less virgin aggregate, and less liquid asphalt. In addition, road life will improve leading to fewer road replacements.

PROJECT HIGHLIGHTS FOR FY 1996

- Potential flaws in the standard SHRP asphalt accelerator-aging test were shown by comparing the ambient- and accelerated-oxidation of commonly used asphalts and asphalt fractions.

- An asphalt aging model was developed that relates the deterioration of physical properties to changes in chemical composition.

- It was verified that recycled-asphalt binders with superior performance-properties could be produced using recycling agents made with supercritical fractions.

- It was established that the single most important factor affecting the properties of recycled asphalt is dilution of the existing asphaltenes present in the aged material.

PARTICIPANTS/PARTNERS

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Dilute Oxygen Combustion System

BACKGROUND

Steel reheating is an energy-intensive process step in making steel products. Steel slabs and blooms are uniformly heated to about 2300º F in a continuous furnace for subsequent hot rolling to semi-finished products. As each steel mill strives to improve productivity, the heating capacity of the reheat furnace often becomes a bottleneck. The expansion of the existing furnace is often constrained by the physical space available, emissions regulations, and the large amount of capital required.

This project is developing the Dilute Oxygen Combustion (DOC) system for use in steel reheating and other furnaces. The DOC system allows for the low cost retrofit of the existing furnace and provides greater heat flux to the steel within the same furnace and with the same flue gas handling equipment.

The basic concept of the DOC system is to burn fuel with very dilute oxidant containing only two to ten percent oxygen to reduce the peak flame temperature and achieve very low NO_x emissions. In combination with the goal of achieving very low NO_x emissions of less than 9 ppm, the DOC system is also expected to provide significant cost savings of 40 to 50 percent fuel savings and 10 to 30 percent production rate increases as compared to conventional combustion systems. In order to create a dilute oxygen stream with the furnace air, oxygen is injected at some distance away from the fuel and mixed with hot furnace gases. High fuel-jet velocities, far exceeding that of the normal flame blow-off velocity with cold air, are used to entrain a large volume of dilute oxidant and to complete combustion reactions. Similarly, high oxygen jet velocities are used to promote sufficient in-furnace recirculation of the oxidant so that no external flue gas recirculation is required.

ENERGY SAVINGS AND ENVIRONMENTAL BENEFITS

By the year 2010, the use of this technology will provide the following annual benefits:

- 8 trillion Btu of energy savings
- 110,000 tons of NO_x emissions avoided
- $2.6 billion in capital expenditures for "end-of-pipe systems."

PROJECT HIGHLIGHTS FOR FY 1996

- Ultra-low NO_x emissions were demonstrated in a laboratory furnace (1 MMBtu/hr). NO_x emissions below 10 ppm at 3% excess oxygen and CO emissions less than 35 ppm were obtained for furnace temperatures below 2,300º F at firing rates of 0.6 MMBtu/hr and furnace nitrogen concentration levels between 1 and 40%. Detailed in-furnace measurements revealed the importance of the interior furnace circulation patterns, as influenced by fuel and oxidant injection schemes, on pollutant emissions.

- Phase I of the DOC project nears completion with encouraging results. Jet entrainment rates were measured as a function of surrounding gas temperature and composition. During Phase II, field testing of a commercial-scale system in a steel reheat furnace is planned.

PARTICIPANTS/PARTNERS

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DIMOX™ (CFCCs)

BACKGROUND

U.S. industry has a critical need for materials that are light, strong, corrosion resistant, and capable of performing in high temperature environments. Although many traditional ceramics perform well at high temperature, they typically fail in a catastrophic manner in service. Continuous Fiber Ceramic Composites (CFCCs) are being developed to overcome this problem by incorporating continuous ceramic fiber into a ceramic matrix. This results in high strength, high temperature materials that exhibit tough behavior.

This project is examining Nicalon™ silicon carbide fiber-reinforced alumina matrix composites made from the Direct Metal Oxidation (DIMOX™) process for industrial applications. These composites will be examined for applications that require good thermal shock resistance, high fracture toughness, and excellent elevated temperature stability. Aluminum oxide fiber-reinforced alumina matrix composites will be considered for resistance to hot and aqueous corrosion, depending on application requirements.

The project will evaluate opportunities for CFCC use in coal-fired combined-cycle power generating systems, in combustor liners for industrial turbine systems, in turbine tip shrouds in fired turbines for utility applications, and in components in hot-gas filtration systems. The components being developed are oxide systems and therefore are resistant to oxidation and corrosion, which will make them well suited for use in the chemical and refining industries.

ENERGY SAVINGS AND ENVIRONMENTAL BENEFITS

By the year 2010, the CFCC program (as a whole) will provide the following annual benefits:

- 600 trillion Btu of energy savings
- 980,000 tons of NO_x emissions avoided
- 119 million tons of CO_2 emissions avoided
- CFCC component sales of \$850 million, adding over 8,000 industrial sector jobs
- Increased industrial process efficiencies, enhanced U.S. industrial competitiveness, and decreased reliance on strategic materials.

PROJECT HIGHLIGHTS FOR FY 1996

- A 100 hour test of the turbine engine combustor liner was completed. This test demonstrated the reliability of the composite and the temperature capability required to continue design work.
- The database was completed for the second generation CFCC system utilizing Hi-Nicalon in a DMO alumina matrix. This system demonstrated a higher design stress capability than the first generation ceramic grade Nicalon. In addition, increased temperature capability and increased lifetime at the higher stress were demonstrated.
- In process modeling efforts with Sandia National Laboratories, a demonstration was completed of a predictive model for uniformity of interface cooling in a part.
- Fareed, Ali. "Mechanical Properties of CFCC's by DIMOX™ Directed Metal Oxidation Process." Presented at the 20th Annual Conference on Composites, Materials and Structures, Cocoa Beach, Florida, January 23-25, 1996.

PARTICIPANTS/PARTNERS

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Emissions (PERF)

BACKGROUND

Toxic combustion by-products, or air toxics, will be regulated in the year 2000 under the Clean Air Act Amendments of 1990. A source of air toxics at petrochemical plants is the air emissions from petrochemical process heaters. These heaters burn refinery fuel gas, a composition of varying amounts of hydrogen, methane, propane, and other hydrocarbons that is an off-product of the refinery process. Refinery fuel gas provides most of the fuel at refineries.

The goals of the project were (1) to assess the state of air toxics emissions in existing burners used in process heaters, (2) to evaluate candidate burners and combustion control strategies that would lessen air toxics generation, and (3) to provide a fundamental understanding of the contributory fluid mechanics, combustion and high-temperature chemistry, and process thermal environments that lead to the production and release of air toxics emissions.

ENERGY SAVINGS AND ENVIRONMENTAL BENEFITS

By the year 2010, this technology will realize the following savings annually:

- 8 trillion Btu of energy savings
- 1,400 tons of air toxics emissions avoided
- 450,000 tons of CO_2 emissions avoided.

PROJECT HIGHLIGHTS FOR FY 1996

- At Sandia National Laboratories (SNL), fundamental experiments were conducted in the flame research laboratory and applied experiments were conducted with industrial burners in the Burner Engineering Research Laboratory (jointly sponsored by DOE and the Gas Research Institute). A key component of the experiments in the Burner Engineering Research Laboratory was an experimental representation of the convective cool-down sections used in process refineries.
- In cooperation with Lawrence Livermore National Laboratory (LLNL), SNL built models of the pertinent chemical submechanisms. At LLNL, chemical kinetics models were built that describe the formation of the air toxics in the combustion zone and their fate as they pass out of the zone and through the convective cool-down section. The University of California at Los Angeles (UCLA) performed fundamental experiments in specially designed and instrumented burners to provide the data for the LLNL chemical kinetics models.

PARTICIPANTS/PARTNERS

SNL, LLNL, UCLA, Stanford University, Southern California Gas, the Gas Research Institute, and Petroleum Environment Research Forum (PERF) members Amoco, Chevron, Mobil, Shell, and Texaco.

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Fouling Mechanisms

BACKGROUND

This ongoing project is developing prediction methodologies for the effects of physical parameters and determining threshold-fouling conditions for processing of petroleum products. Since 1994, the project has focused on developing new and improved methods to mitigate fouling in preheat train heat exchangers in crude oil distillation, and in feed/effluent heat exchangers in hydrotreating processing.

The major objectives for the project are to determine the major causes of fouling, to develop methodologies for predicting threshold conditions for different feedstocks, and to develop new techniques to improve the effectiveness of chemical additives that prevent fouling deposition. The project has three components: 1) development of a prediction model that incorporates kinetic and fluid dynamic models, 2) laboratory experiments to develop kinetic models for the formation of fouling precursors, and 3) field experiments to validate the laboratory data.

ENERGY SAVINGS AND ENVIRONMENTAL BENEFITS

The overall energy efficiency of refineries is dependent on the feed/effluent heat exchangers that recover thermal energy from high temperature processes. Fouling buildup impedes heat transfer, and the lost energy must be supplied by furnaces using gas or liquid fuels. The resulting economic and energy costs for the U.S. refineries are well known: 0.2 quads of energy and more than $2 billion are lost each year due to fouling. The fouling problem in the petroleum refining industry is becoming critical due to increased use of heavy oil and residuum.

PROJECT HIGHLIGHTS FOR FY 1996

- Two field-fouling monitor units were installed at the Shell Wood River Refinery for crude distillation and at the Chevron El Segundo Refinery for hydrotreating processes.
- A design method was developed to accurately predict onset conditions of fouling with hydrocarbon fluids.

PARTICIPANTS/PARTNERS

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Heat Management Equipment through CVI (CFCCs)

BACKGROUND

U.S. industry has a critical need for materials that are light, strong, corrosion resistant, and capable of performing in high temperature environments. Although many traditional ceramics perform well at high temperature, they typically fail in a catastrophic manner in service. Continuous Fiber Ceramic Composites (CFCCs) are being developed to overcome this problem by incorporating continuous ceramic fiber into a ceramic matrix. This results in high strength, high temperature materials that exhibit tough behavior.

As part of the DOE's CFCC program, this project is fabricating and testing CFCC materials manufactured from silicon carbide through chemical vapor infiltration (CVI) for industrial applications. DuPont Lanxide is developing CVI of silicon carbide CFCC components and incorporating the components into a variety of high-temperature, heat management, and power generation equipment.

The project team has assessed which applications will most benefit from the use of CFCC components, and has identified the performance and economic targets for initial applications. Additional applications are being identified for continued assessment as data from successful tests are made known industry wide. The team is now fabricating, exposing, and testing CVI CFCC materials in simulated and actual applications conditions to prove their suitability for the selected applications. The components being developed have excellent potential benefits for high temperature and high erosion applications. Of particular interest are radiant burners for the chemical industry. Other components having cross-cutting applications, such as heat exchangers and turbine components, are going into field testing at industrial sites for 4000 and 8000 hour tests.

ENERGY SAVINGS AND ENVIRONMENTAL BENEFITS

By the year 2010, the CFCC program (as a whole) will provide the following annual benefits:

- 600 trillion Btu of energy savings
- 980,000 tons of NO_x emissions avoided
- 119 million tons of CO_2 emissions avoided
- CFCC component sales of $850 million, adding over 8,000 industrial sector jobs.

PROJECT HIGHLIGHTS FOR FY 1996

- CFCC components were identified that would help increase the power generation efficiency of a coal-fired power plant from 35% to 47% with a 25% reduction in emissions.
- Two applications were identified for near-term commercialization: hot gas filters and porous radiant burners.
- Highly permeable CFCC plates and tubes were developed and tested for specific applications. Flat plate radiant burner screens have been tested for 15,000 thermal cycles.
- Headinger, Mark and Jim Weddell. "The Influence of Nicalon™ Fiber Volume in Enhanced SiC/SiC Composites." Presented at the 20th Annual Conference on Composites, Materials and Structures, Cocoa Beach, Florida, Jan. 23-25, 1996.

PARTICIPANTS/PARTNERS

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High Temperature Catalytic Membrane

BACKGROUND

Organic chemicals - those containing the element carbon - are produced from petroleum and natural gas in refineries and other chemical production facilities. Most chemical production processes require the input of thermal energy (usually in the form of steam) to carry out the desired chemical reactions and separations. The yield of these reactions is often limited to 50 percent or less, which means that the process must be repeated several times to get the desired amount of product. The dehydrogenation (removal of the hydrogen) from the chemical ethylbenzene to produce the chemical styrene provides a good example of the problems associated with conventional thermal processing. This reaction requires high temperatures (and thus a lot of energy) and an expensive catalyst, but the yield is low and the reactor vessel takes a terrible beating.

A membrane separation process that uses a porous ceramic membrane impregnated with a catalyst has been developed for use in the conversion of ethylbenzene to styrene. In the new membrane reactor, the unwanted hydrogen radiates outward through the tubular membrane, while the desired styrene component passes straight down the center and out the other end for further processing. Because the hydrogen is removed through the membrane wall as it is formed, it cannot re-react with the styrene to produce the original ethylbenzene again, a problem that lowers the conversion rate of the conventional process.

The project's objective is to develop membrane modules that can increase the efficiency and lower the processing temperatures of dehydrogenation for processing styrene, ethylene, isobutane, and other dehydrogenation reactions.

ENERGY SAVINGS AND ENVIRONMENTAL BENEFITS

By the year 2010, the use of this technology (50 operating units) will provide the following annual benefits:

- 4.5 trillion Btu of energy savings in the production of styrene from ethylbenzene, and 2 trillion Btu in the production of isobutylene from isobutane.
- Reduced temperature operation and catalyst fouling, which increases the length of efficient catalyst use and significantly decreases the amount of hazardous waste generated.

PROJECT HIGHLIGHTS FOR FY 1996

- A high temperature screening unit (STU) was designed and built at Chevron to evaluate hydrogen selective membranes.
- Three membrane technologies were evaluated in STU for their ability to separate hydrogen from hydrocarbons at high temperatures (Palladium, CVD Silica, Silicate Zeolite).
- The ability of two membrane technologies (Silica and Palladium) to efficiently remove hydrogen from propane at high temperatures was demonstrated.
- A method to infiltrate ceramic substrates with metal for a high temperature seal was demonstrated.
- The project team designed and initiated development of methods to braze ceramic/metal infiltrated end seals to metal end pieces.

PARTICIPANTS/PARTNERS

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Life-Cycle Computer-Aided Data Project

BACKGROUND

In the face of customers' demands for environmentally friendly products and regulatory and societal pressures for environmental friendly operations, many companies are realizing the tremendous opportunity that exists in strategies that integrate energy and environmental considerations into all business practices. These companies find that adopting an integrated strategy provides a competitive advantage in U.S. and global markets and positions them strategically for the next century, when aggressive energy and environmental management will be imperative for survival.

Such an integrated strategy requires data and decision frameworks that enable decision makers to evaluate the lifetime (cradle-to-grave) energy and environmental impacts of a technology. Within industry and government, life-cycle assessment (LCA) is increasingly recognized as a key approach for these business evaluations.

Two difficulties associated with integrating LCA into standard business practices are a lack of standardized LCA tools and a lack of standardized data sets. The lack of these tools and data makes widespread, consistent, and cost-effective use of LCA virtually impossible. This project seeks to develop the needed LCA tools and data sets.

PROJECT HIGHLIGHTS FOR FY 1996

- Prototype LCA software was completed.
- Beta test license agreements were signed with fifteen trade associations, companies, and universities.
- A commercialization agreement was reached with Battelle Memorial Institute.

PARTICIPANTS/PARTNERS

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OFFICE OF INDUSTRIAL TECHNOLOGIES
Productivity through Technology

Low-Temperature Catalytic Gasification of Chemical Manufacturing Wastewater

BACKGROUND

The chemical manufacturing industry is in need of appropriate technology for the disposition of organic chemical contaminated wastewater. The organic chemical manufacturing industry currently uses deep-well injection for disposing of over 15 million gallons per day of hazardous organic chemical containing wastewater. The purpose of this project is to facilitate the development of the Thermochemical Environmental Energy System (TEES)® concept to convert wet industrial wastes to significant quantities of methane in order to provide energy conservation, reduced environmental impact from disposal of wastewater, and improved process economy because of both effects. TEES is a unique thermocatalytic gasification concept that converts organic chemicals in wastewater to methane and carbon dioxide (for use as medium-Btu fuel gas); cogeneration, waste water treatment, and reduction in solid waste handling can also be achieved. The catalytic system operates at high pressure (20 MPa) and low temperature (300-350^{o} C) compared with conventional gasification approaches. The project has a full range of process development systems, from a small batch reactor to a bench-scale continuous-flow research unit to a scaled-up engineering development unit.

ENERGY SAVINGS AND ENVIRONMENTAL BENEFITS

By the year 2010, the use of this technology will provide the following annual benefits:

- 6.4 trillion Btu of energy savings
- 11.1 million tons of waste reduction
- 0.39 million tons CO_2 emissions avoided.

The energy generated is the net gas product produced from waste organics. The waste includes both landfilled waste and wastewater, including hazardous wastewater.

PROJECT HIGHLIGHTS FOR FY 1996

- The production of new generation catalysts was demonstrated by BASF.
- U.S. patents covering next generation catalysts and broad chemical processing applications are pending.

PARTICIPANTS/PARTNERS

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Motor Challenge

BACKGROUND

More than one billion electric motors are currently used in industrial, commercial, residential, and utility power plant applications in the United States. U.S. industry spends roughly $30 billion annually on electricity to drive motor systems. The Motor Challenge program is a joint effort of DOE, industry, equipment manufacturers and distributors, and other interested parties to promote integrated systems of energy efficient motors, adjustable speed drives, and efficient motor-driven mechanical equipment and processes. As part of President Clinton's Climate Change Action Plan, Motor Challenge is recognized as representing a significant opportunity to enhance environmental performance and reduce energy consumption in U.S. industry.

The overall goal of the Motor Challenge initiative is to advance industry leadership and provide technical assistance and resources to industry so that firms will better understand, apply, and target energy efficient electric motor systems (EMS) from a systems perspective. In most cases, the technology already exists to use efficient EMS. Motor Challenge was designed to act as a catalyst to foster broad-based industrial participation in exchanging information and deploying technology. DOE has worked diligently with stakeholders to identify barriers and opportunities related to adopting more efficient EMS. The program works with partners to focus on deficiencies in the market that influence choices of stakeholders in specifying, purchasing, and operating equipment and that impede development and introduction of better products and services. Motor Challenge consists of five elements: 1) Showcase Demonstrations; 2) Allied Partnership; 3) Industry Partnership; 4) Excellence Partnership; and 5) Information Clearinghouse.

ENERGY SAVINGS AND ENVIRONMENTAL BENEFITS

By the year 2010, the Motor Challenge program will assist industry in realizing the following annual benefits:

- 6.89 billion kWh of electricity savings
- 1.1 million metric tons of carbon equivalent emissions avoided.

PROJECT HIGHLIGHTS FOR FY 1996

- Over 590 new Motor Challenge partners joined the program. Over 58 industry organizations joined the Alliance Partnership.
- The MotorMaster+ software was released; the on-line training program has certified over 200 users.
- 10 Performance Optimization Workshops focusing on water/wastewater pumping systems were held, reaching 1000 industry representatives.
- Over 5200 requests were processed by the Information Clearinghouse, which was averaging 600 calls per month at the end of FY 1996.
- 11 new showcase demonstration projects were added to the program, bring the total to 29. Completed projects have validated annual energy savings totaling $1.2 million.
- 4 new training modules related to electric motor-driven systems were released.
- Ads promoting the Motor Challenge program appeared in seven industry publications.
- A feature article prepared by the Motor Challenge program and the Hydraulic Institute, "Energy-Efficient Pumping Systems," appeared in the August 1996 issue of *Chemical Processing*.

PARTICIPANTS/PARTNERS

The Motor Challenge program has over 1,600 partners. Among these are: DuPont, Dow Chemical, General Electric, Hoechst Celanese, Nalco Chemical, Pratt & Lambert, R.C. Cement, Raffi-Swanson, Johnson & Johnson, Enron, Eastman Kodak, Warner-Lambert, Nova Chemical, Carpenter Company, Roche Vitamins & Fine Chemicals, Ayerst-Wyeth Pharmaceuticals, Jafra Cosmetics International, Chemical Processing, and the Chemical Manufacturers Association.

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National Center for Manufacturing Sciences Cooperative Agreement

BACKGROUND

The National Center for Manufacturing Sciences (NCMS) is a consortium of manufacturers formed in 1986. NCMS is committed to making North American manufacturing globally competitive through the development and implementation of next-generation technologies. Recognizing the links between manufacturing competitiveness, economic growth, and environmental respect, NCMS established the NCMS Environmentally Conscious Manufacturing (ECM) Program to identify and solve major industrial environmental problems through collaborative efforts among leading American manufacturers, government agencies, academia, and other organizations.

The DOE has established a cooperative agreement with NCMS to research and develop innovative pollution prevention technologies in collaboration with NCMS and industrial sponsors and to catalyze the adoption of pollution prevention technologies through education, training, and technology transfer activities. The agreement provides the OIT with a critical manufacturing sector resource for implementing Industry Visions, particularly the chemical and metal casting industry visions.

Multiple projects will be sponsored under the NCMS Cooperative Agreement. Projects underway include the following:

- Prediction of Foundry Emissions
- Mass Flow Controller for Zero Solvent Coatings
- Precision Forging for the Manufacture of Complex Shapes

PARTICIPANTS/PARTNERS

The NCMS and its members, which include Advanced Processing Technology, Inc., the American Plastics Council, American Propylaea Corp., the Association for Manufacturing, Eastman Kodak Co., Flavors Technology, Inc., the Great Lakes Composites Consortium, the High Performance Manufacturing Consortium, the Independent Lubricant Manufacturers Association, Johnson Manufacturing Company, Light Machines Corporation, Manufacturing Resources, Inc., the Michigan Biotechnology Institute, Midwest Manufacturing Technology Corporation, Performance Controls, Inc., United Technologies Corporation, and Westinghouse Electric Company.

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Polymer Impregnation and Pyrolysis (CFCCs)

BACKGROUND

U.S. industry has a critical need for materials that are light, strong, corrosion resistant, and capable of performing in high temperature environments. Although many traditional ceramics perform well at high temperature, they typically fail in a catastrophic manner in service. Continuous Fiber Ceramic Composites (CFCCs) are being developed to overcome this problem by incorporating continuous ceramic fiber into a ceramic matrix. This results in high strength, high temperature materials that exhibit tough behavior.

This project is an industrial team effort to develop CFCCs for industrial applications using the polymer impregnation and pyrolysis (PIP) process. The PIP process is a versatile method of fabricating large, complex-shaped structures. The material produced, SYLRAMIC™ composite, exhibits both high strength and tough behavior up to 1200° C.

The CFCC applications being considered are (1) gas turbine combustor liners and interstage seals, (2) chemical pump components, and (3) pipe hangers for oil refinery furnaces. The chemical pump components and pipe hangers will be useful to both the chemical and refining industries.

ENERGY SAVINGS AND ENVIRONMENTAL BENEFITS

By the year 2010, the use in industrial applications of the CFCCs developed under this project will provide the following estimated annual savings:

- As much as $1.9 billion in energy cost savings
- Up to 500,000 tons of NO_x emissions avoided
- Up to 70 million tons of CO_2 emissions avoided.

PROJECT HIGHLIGHTS FOR FY 1996

- Fabrication of a combustor liner, pipe hangers, and a containment shell was successfully demonstrated for evaluation.
- A SYLRAMIC™ S200 composite sub-scale combustor liner was successfully tested for 100 hours in a combustor rig at Solar Turbines.
- SYLRAMIC™ S200 CFCC coupons were demonstrated to retain strength and toughness after 8,400 hours of exposure to 1,800-2,000° F temperatures in an oil refinery environment.
- The fiber architecture was selected for fabrication of a chemical pump component.
- The stability of CFCC in organic and inorganic chemicals was demonstrated at elevated temperatures.

PARTICIPANTS/PARTNERS

Dow Corning Corporation, Chevron Research & Technology Company, Kaiser Compositek, Solar Turbines, Sundstrand Aerospace, Sundstrand Fluid Handling, and Synterials, Inc.

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Production of Ethanol from Refinery Waste Gases

BACKGROUND

Refineries discharge large volumes of H_2, CO, and CO_2 from cracking, coking, hydrotreating, and other operations. A typical refinery producing 200,000 barrels per day (BPD) discharges 324,000 tons of waste H_2 and CO per year. This research program is developing a biological process for the conversion of these waste gases into ethanol, which can be blended with gasoline to increase octane and reduce emissions. A 200,000 BPD refinery could produce 58 million gallons of ethanol per year and generate about $75 million annually from the waste gases. The technology does not require purification of the gases and no modifications to existing processes are required. Preliminary economics show that ethanol can be produced for substantially less than the current grain alcohol price.

ENERGY SAVINGS AND ENVIRONMENTAL BENEFITS

By the year 2010, the use of this technology will provide the following annual benefits:

- 450 trillion Btu of energy savings
- 110 million barrels of reduced crude oil imports
- 19 million tons of H_2, CO and CO_2 emissions avoided.

PROJECT HIGHLIGHTS FOR FY 1996

- It was demonstrated that the fermentation unit for converting CO, CO_2, and H_2 refinery waste gases to ethanol can operate without interruption for more than 12 months.

- The continuous operation of the bench-scale ethanol production unit was demonstrated, including fermentation, cell removal, distillation, and water recycle.

- The design of a pilot plant for the conversion of refinery waste gas to ethanol at production rates of up to 2.5 lb/hr of ethanol was completed.

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Selective Oxidation Catalysis

BACKGROUND

This effort seeks to develop experimental and theoretical tools to study heterogeneous catalysis. Research focuses on development of novel solid-state formalism, its application to zeolites and clays, and experimental validation of molecular-level processes in commercial catalytic reactions. For the study of the molecular-level aspects of homogeneous catalysis, there exists a relatively large tool kit that can be used to probe the catalyst system for information about structure, dynamics, and reaction mechanisms, including vibrational spectroscopy, molecular quantum chemistry, and NMR. However, when studying the molecular-level events in a heterogeneous system with an external or internal surface, the number of useful tools is considerably diminished due to the complexity of the physics.

This project is pursuing the development of several tools aimed at facilitating the study of solid-state structure in heterogeneous catalysts. These include the development of periodic *ab initio* Hartree-Fock theory and its application to aluminosilicates and metal oxides, and the formation of a model to describe the phenomenon of "site isolation" in selective oxidation catalysts. Improvements are sought that are clearly revolutionary relative to current practice or understanding and not just incremental.

PROJECT HIGHLIGHTS FOR FY 1996

- Development and testing of the spin paired and spin polarized 3- and 2-dimensionally periodic total energy models were completed for the GAPSS (Gaussian Approach to Polymers, Surfaces, and Solids) program. GAPSS has been designed to operate efficiently on massively parallel computers and uses the NWCHem suite programs as a backplane. Both GAPSS and NWCHem operate efficiently (scaling to hundreds of nodes) on both distributed and shared memory architectures.
- The total energy modules of the self-consistent solutions of the Kohn-Sham equations, yielding total energies for simple bulk crystalline systems (MgO, diamond, silicon, and SiC) were completed in January 1996. Subsequently, the geometries, elastic moduli, and electronic structures of a wide range of insulating and semi-conducting materials have been studied.
- The total energy surface modules (capable of treating systems periodic in two dimensions) for both spin paired and open shell systems were completed in March 1996. The modules have since been used to study a range of oxide (MgO, CaO, SiO_2, etc.) and transition metal oxide (MnO, FeO, and NiO) surfaces with and without simple (e.g., CO, NO, and H_2O) molecular adsorbates.
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PARTICIPANTS/PARTNERS

Pacific Northwest National Laboratory (PNNL), Catalytics, Exxon, Phillips, AlliedSignal, DuPont Co., and Amoco.

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Solar Detoxification

BACKGROUND

Photocatalytic oxidation (PCO), also known as photo detoxification, uses energy in light to destroy environmental contaminants. Applicable as both a waste clean-up and a pollution control technique, PCO could help thousands of businesses, large and small, comply with environmental regulations. The PCO process uses a photoactive catalyst, such as titanium dioxide, which catalyzes chemical reactions in the presence of ultraviolet light. The chemical bonds of toxic organic pollutants break down, converting the toxic compounds to carbon dioxide and water. PCO is effective in destroying contaminants such as solvents, dyes, fuel oils, and other industrial wastes. It can control pollution at the source, such as air and water emissions, or clean it up afterwards, as in the case of contaminated groundwater. The process is most effective when used to treat low concentration, low-flow-rate waste streams.

This project seeks to further develop PCO processes to the point of successful commercialization for waste treatment and pollution prevention. The first field demonstration of solar PCO will take place in 1997.

ENERGY SAVINGS AND ENVIRONMENTAL BENEFITS

By the year 2010, the use of this technology will provide the following annual benefits:

- 107 trillion Btu of energy savings
- 7.1 million tons of CO_2 emissions avoided
- Over 100 million dollars in cost savings.

PROJECT HIGHLIGHTS FOR FY 1996

- Experiments and the Phase 2 report were completed for the SEMATECH project to evaluate PCO for air emission abatement from semiconductor manufacturing.
- The final design for gas phase photoreactors to be demonstrated at a Department of Defense (DOD) site in 1997 was developed.
- The final report on new processes for treating water contaminated with explosives for the SERDP program was submitted.
- Successful field tests of a PCO process for treating paint booth emissions were carried out at two DOD sites.
- Jacoby, W.A., D.M. Blake, J.A. Fennell, J.E. Boulter, L.M. Vargo, M.C. George, and S.K. Dolberg. 1995. "Heterogeneous Photocatalysis for Control of Volatile Organic Compounds in Indoor Air." *J. Air and Waste Management Assoc.*, **46**: 891-898.
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PARTICIPANTS/PARTNERS

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Theoretical Studies of Hydrocarbon Catalysts

BACKGROUND

This project develops computational tools to model chemical transformations of small hydrocarbon molecules within zeolite catalysts. In addition, it coordinates catalysis-by-design activities for inorganic catalysts and conducts an experimental program to provide verified, generic tools for catalysts of interest to industry.

In this project, catalyst research has focused on the details of carbon-carbon bond formation within the pentasil zeolite, ZSM-5. This catalyst has special significance for energy applications; for example, it is used in the "methanol-to-gasoline" process, and has many uses in conventional petroleum cracking. Pentasil zeolites provide unmatched shape selectivity for hydrocarbon molecules; hydrocarbon molecular weight produced within zeolite cannot exceed the limit of light hydrocarbons of gasoline fractions.

Many of the details of the catalytic processes are unclear, however, and warrant fundamental investigations if their yield and selectivity are to be improved, and is energy to be saved, in these processes. These details include the nature of the acid sites responsible for catalysis and transport properties such as absolute diffusivities. Models of the adsorption and bond formation processes within zeolites will be derived by classical (molecular-dynamics), quantum, and quantum-statistical methods.

Catalyst research will also include modeling and experimental studies of metal oxide oxidations of hydrocarbons. These case studies were suggested by industrial collaborators of the project. Specific project technical objectives include the following: 1) prediction of the chemical state and the role of alumina in zeolite catalysis, and verification of the predictions by X-ray absorption; and 2) use of solid-state ionic conducting ceramics to study hydrocarbon oxidations using new experimental techniques to control the surface free energy.

PROJECT HIGHLIGHTS FOR FY 1996

- Calculations were carried out of the vibration frequencies of carbon monoxide and nitric oxide in cluster models of zeolite Cu-ZSM-5. These zeolites have been found to have enhanced activity for the catalytic decomposition of NO_x in the presence of hydrocarbons and excess oxygen.

PARTICIPANTS/PARTNERS

Los Alamos National Laboratory (LANL), W.R. Grace, Shell, Exxon, Merck, and Arco Chemical.

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Theory-Assisted Design of Metal and Zeolite Catalysts

BACKGROUND

The project will develop and validate a hierarchy of theoretical models that could be used by industry for the design and development of zeolite catalysts. Catalyst properties (enthalpies and entropies of adsorption and formation and other thermodynamic parameters) will be calculated and compared with known experimental values. The overall goal is a complete description of various industrially relevant heterogeneous catalyst systems, with models of increasing degrees of sophistication. These models will allow increasingly better prediction of industrially important phenomena, which can be used for the design of zeolite-based catalysts.

PROJECT HIGHLIGHTS FOR FY 1996

Zeolite Catalysts

- The structure and thermodynamics of adsorbed species involved in the decomposition of NO over CU-ZSM-5 were determined using a combination of density functional theory and statistical mechanics. With this information, alternative pathways for NO decomposition have been examined. It was concluded that it is thermodynamically feasible for NO decomposition to take place over single CO cations. The results of these calculations are in good agreement with experimental findings.

Diffusion in Zeolites

- Development was completed on a model for the diffusion of long-chain alkanes in zeolites, based on Brownian Dynamics and Transition State Theory. This model is one to three orders of magnitude more efficient than molecular dynamics simulations and provides estimates for self-diffusion coefficients that are of comparable accuracy. The predicted dependence of the diffusion coefficient for n-alkanes in the range of C_5 - C_{20} is in good agreement with that observed experimentally.

Zeolite Synthesis

- A protocol was developed for estimating the enthalpy and Gibbs free energy change for the synthesis of highly siliceous zeolites starting from the amorphous silica and an aqueous solution of the structure-directing agent (i.e., tetraalkylammonium hydroxide, TAAOH). Using this approach, the effects of cation composition and the extent of occlusion on the synthesis of ZSM-11 were investigated. It was found that, in agreement with experiment, ZSM-11 is synthesized most effectively starting from tetrabutylammonium hydroxide rather than tetrapropylammonium hydroxide.

- Trout, B.L., A.K. Chakraborty and A.T. Bell. 1996. "Local Spin Density Functional Theory Study of Copper Ion-Exchanged ZSM-5." *J. Phys. Chem.*, **100**: 4173.

PARTICIPANTS/PARTNERS

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Toughened Silcomp (CFCCs)

BACKGROUND

Current gas turbines used in power generation applications (excluding marine and aircraft applications) have large cooling requirements, typically requiring 30 to 40 percent of their discharge air for component cooling. This lowers the energy efficiency of the turbine, thus increasing its fuel requirements. Replacing metal alloy components with continuous fiber ceramic composite (CFCC) components could substantially increase this energy efficiency by allowing the turbine to operate at higher temperatures. The problem to date has been developing a CFCC and a corresponding fabrication method that could be used to make the components in the required shapes.

As part of OIT's CFCC Program, a new material called Toughened Silcomp has been developed for just such applications. Toughened Silcomp consists of a continuous network of silicon carbide fibers within a silicon-silicon carbide matrix. This material and its fabrication technique -known as melt infiltration - can be used to produce a variety of fully dense, complex-shaped parts. The material's density gives the composite good oxidation resistance, high thermal conductivity, low thermal expansion, and good strength, all desirable characteristics for gas turbine applications.

ENERGY SAVINGS AND ENVIRONMENTAL BENEFITS

By the year 2010, the CFCC program (as a whole) will provide the following annual benefits:

- 600 trillion Btu of energy savings
- 980,000 tons of NO_x emissions avoided
- 119 million tons of CO_2 emissions avoided
- CFCC component sales of $850 million, adding over 8,000 industrial sector jobs.

PROJECT HIGHLIGHTS FOR FY 1996

- The feasibility of using fiber coatings from two commercial vendors for composites reinforced with Hi-Nicalon Fibers was demonstrated.
- Test techniques for identifying environmental embrittlement problems with ceramic components were developed.
- Potential problems with Boron Nitride fiber coatings in water vapor environments were identified.
- The feasibility of an oxidation resistant fiber coating in Hi-Nicalon fiber reinforced SiC-Si matrix composites was demonstrated.
- Corman, G. and K. Luthra. December 1996. "Improved Properties of Gas Turbine Engine Components Utilizing CFCC and Melt Infiltration." *Industrial Heating*, **LXIII**(12).
- Corman, G.S., K.L. Luthra, and M.K. Brun. "Toughened Silcomp (SiC-Si) Composites for Gas Turbine Engine Applications: CFCC Phase 2 Status." Presented at the 20th Annual Conference on Composites, Materials, and Structures, Cocoa Beach, FL, January 23-25, 1996.

PARTICIPANTS/PARTNERS

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Environmental Technology Partnership Program R&D

The Department of Energy (DOE) and the National Science Foundation are joint sponsors of the Environmental Technologies Partnership (ETP) program, which supports research and development on cleaner technologies and policies for the seven "Industries of the Future" targeted by the DOE's Office of Industrial Technologies. The program addresses the industries' most pressing environmental challenges and is intended to help these industries move from a clean-up and waste management focus to a pollution prevention strategy over the next 5 to 10 years.

Over fifty ETP projects were funded in FY 1996; more than half of these projects address directly or are relevant to the chemical industry. The chemicals and chemicals-related projects are listed and described briefly below. Please contact Brian Volintine at (202) 586-1739 for more information.

- ***Arabidopis Genome Sequencing Using Random Shotgun Sequencing of BAC Clones***. J. Craig Venter, Institute for Genomic Research. This project involves basic research in bioscience aimed at improved plants for energy applications.

- ***Autotrophic Biofilms for Removing Contaminates from Industrial Wastewater***. Walter Hill, Oak Ridge National Laboratory. This project involves basic research in environmental and bioscience aimed at improved remediation of wastewater.

- ***Bimetallic Complexes as Methanol Oxidation Catalysts***. Lisa McElwee-White, University of Florida. This project involves basic research in chemistry and catalysis aimed at improved conversion of chemicals and electrical generation. The work will investigate bimetallic Pt/Ru and Pt/Mo complexes as model compounds for active sites on platinum anodes in direct methanol fuel cells. The ultimate goal of the work is to seek chemically modified electrodes with improved capabilities for electro-oxidation of alcohols.

- ***Bimetallic Oxycarbides and Oxynitrides: A New Class of Hydrogenation Catalysts***. S. Ted Oyama, Virginia Polytechnic Institute. This project involves basic research in chemistry and catalysis aimed at improved hydrogenation catalysts. The goal of the work is to gain a fundamental understanding of the catalytic properties of unique bimetallic catalysts composed of transition metal carbides and nitrides in hydrogenation of aromatic compounds. The work will attempt to achieve significant improvements in catalysts for aromatic hydrogenation.

- ***Carbon Dioxide Based Solvents for Waste Minimization***. Keith Johnston, University of Texas-Austin. This project involves basic research in chemistry aimed at improved use of supercritical carbon dioxide in chemical synthesis. The projects goals include developing new chemical strategies for the design of surfacants for both organic and aqueous interfaces with carbon dioxide.

- ***Clean Solvent Extraction Using Polyethylene Glycol-Based Aqueous Biphasic Systems***. Robin D. Rogers, University of Alabama. This project involves basic research in chemistry, studying new ways to separate chemical compounds from mixtures. The goal of the work is to achieve a fundamental understanding of the factors governing the partitioning behavior of organics in aqueous biphasic separation systems. The work seeks to achieve significant improvements in separations through improved knowledge of these factors.

- ***Computational Thermochemistry***. David Dixon, Pacific Northwest National Laboratory. This project involves basic research in computational science and chemistry aimed at improving efficiency in chemicals manufacture and refining.

- ***Design and Construction of Main Group Element Containing Molecules and Molecule Derived Materials with Unusual Electronic Properties***. B.N. Diel, Midwest Research Institute. This project involves basic research in materials science aimed at the development of improved chemicals for the preparation of advanced thin film semiconductors and other materials.

- ***Enhancement of Lifecycle Analysis using Economic Input-Output Techniques***. Lester Lave, Carnegie-Mellon University. This project involves basic research in environmental research aimed at optimizing value in lifecycle analysis.

- ***Fundamental Studies of C2-C4 Alkane Oxidation Over Model Supported Vanadia Catalysts***. I. Wachs, Lehigh University. This project involves basic research in chemistry and catalysis aimed at improved catalytic conversion of small hydrocarbons. The project will investigate the fundamental aspects of alkane oxidation chemistry over well characterized vanadia catalysts. The goals of the work include developing a fundamental understanding of the molecular structure-reactivity/selectivity relationships that influence the oxidation of alkanes on vanadia catalysts.

- ***Fundamental Studies of Oxygen Storage Materials***. Charles Peden, Pacific Northwest National Laboratory. This project involves basic research in chemistry and catalysis that is aimed at improved catalysts for manufacture and emissions control. The goal of the work is to fill a gap in the fundamental understanding of catalyst activity and durability with respect to the transient NO_x reduction performance in automotive catalytic converters. Ultimately, this detailed understanding will lead to the ability to model both the performance and durability of catalysts in actual vehicles.

- ***Gel for Molecular Recognition and Release***. T. Tanaka, Massachusetts Institute of Technology. This project involves basic research in materials science aimed at gels for selective absorption.

- ***Halocarbon Separations with Zeolitic Materials***. Anthony K. Cheetham, University of California, Santa Barbara. This project involves basic research in chemistry, studying new ways to separate organic compounds containing halogens from mixtures. The work will attempt to achieve significant improvements in separations through improved knowledge of the nature of the factors that control adsorption in zeolites.

- ***Improving Resource Utilization and Pollution Prevention in Plastics Processing***. Jack Killion, Stevens Institute of Technology. This project involves basic research in materials science aimed at improved efficiency in plastics manufacture.

- ***Intrinsic Bioremediation of Gas Condensate Hydrocarbons***. Kerry Sublette, University of Tulsa. This project involves basic research in biosciences and environmental science in bioremediation.

- ***Laboratory Investigation of Constitutive Properties***. Vincent C. Tidwell, Sandia National Laboratories. This project involves basic research in geosciences aimed at improved understanding of fluid behavior.

- ***Multicomponent Convection in Porous Media***. Harlan W. Stockman, Sandia National Laboratories. This project involves basic research in geosciences aimed at improved understanding of convection in porous media.

- ***A New Approach for the Characterization of Buried Interfaces***. Thomas Furtek, Colorado School of Mines. This project involves basic research in materials science aimed at new ways to observe obscured structure in microscopic detail.

- ***Optimization of Chemical Process Heaters and Combustion Systems***. Phillip Smith, University of Utah. This project involves basic research in computational and combustion sciences aimed at more efficient process heaters.

- ***A Parallel Computer Model and Integrated Visualization System for Assessing the Migration of Industrial Mixed Waste Plumes***. Phillip Jardine, Oak Ridge National Laboratory. This project involves basic research in computational sciences aimed at improved remediation of water pollution.

- ***Phase Behavior of Ethylene Copolymer Systems Underlying Energy and Product Wastes Due to Fouling***. Mark Radosz, Louisiana State University. This project involves basic research in chemistry and materials science aimed at improved plastics manufacture.

- ***Plasma Assisted Catalytic Decomposition of NO_x***. Bernie Penetrante, Lawrence Livermore National Laboratory. This project involves basic research in chemistry, catalysis, and plasma physics for improved catalytic destruction of noxious oxides of nitrogen formed in combustion and chemical manufacturing. The work will 1) explore the effects of a plasma on the NO_x reduction activity and temperature operating window of various catalytic materials, and 2) develop a fundamental mechanistic understanding of the interaction between the gaseous-phase plasma chemistry and the heterogeneous chemistry on catalyst surfaces.

- ***Selective Conversion of Light Hydrocarbons to Fuels and Chemicals***. Alexis Bell, Lawrence Berkeley National Laboratory. This project involves basic research in chemistry and catalysis for improved catalytic means of making fuels and chemicals. The work will 1) seek to understand how to control the oxidative dehydrogenation of methane and C_{10} alkanes over both heterogeneous and homogeneous catalysts, and 2) investigate the photo-oxidation of alkanes and alkenes with NO_2 under mild conditions to achieve high selectivity to oxygenated products. Visible light-driven alkane oxidation by O_2 in cation-exchanged zeolites will be explored for the direct conversion to alcohols.

- ***Soil Remediation Strategies and Endpoints***. Brent Peyton, Pacific Northwest National Laboratory. This project involves basic research in environmental science aimed at improved remediation of pollution.

- ***A Study of the Reactions of Hydrofluorocarbons and Hydrochlorofluorocarbons over Basic Zeolites***. Clare Grey, State University of New York-Stony Brook. This project involves basic research in chemistry and catalysis aimed at the catalytic destruction of chlorofluorocarbons.

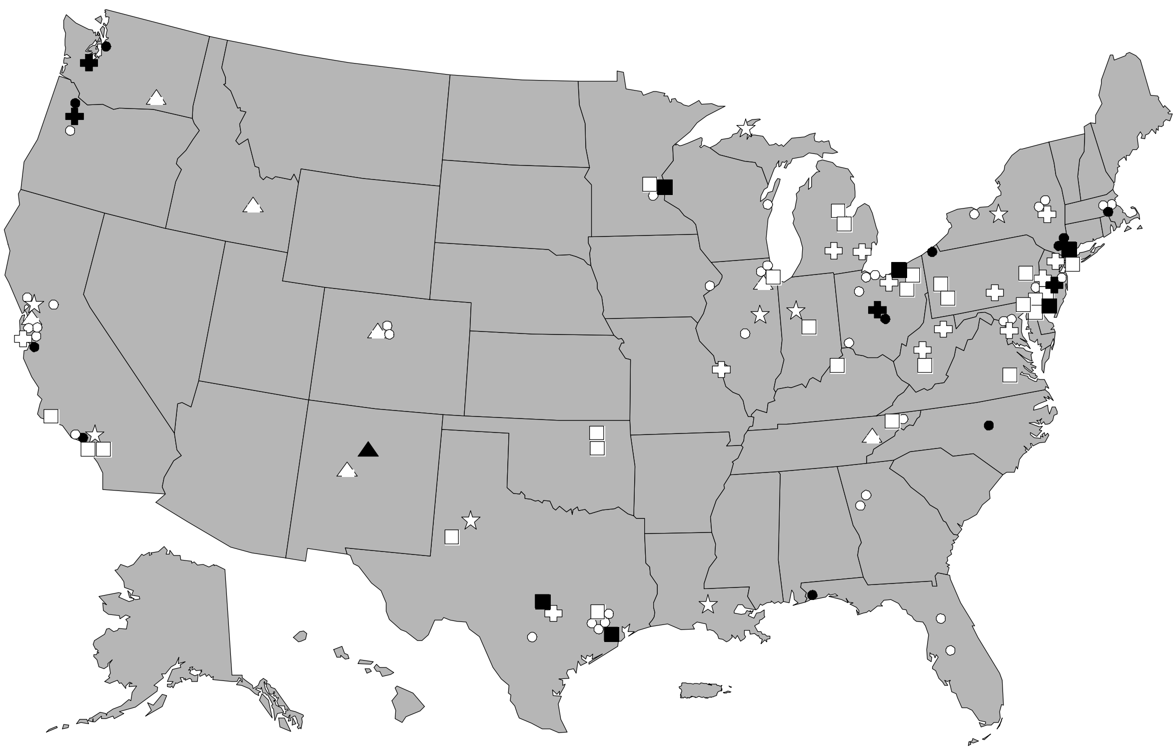
- ***Two-Phase Immiscible Fluid Flow***. Robert J. Glass, Sandia National Laboratories. This project involves basic research in geosciences aimed at improved understanding of fluid flow.

- ***Understanding and Controlling Metal-Support Interactions in Nanocrystalline Bimetallic Catalysts***. James Howe, University of Virginia. This project involves basic research in chemistry and catalysis aimed at improved environmental catalysts. The work will attempt to achieve a fundamental understanding of the catalytic properties of bimetallic nanocrystalline catalysts as a function of their allow composition and interactions with the catalyst support.

OFFICE OF INDUSTRIAL TECHNOLOGIES
Productivity through Technology

CHEMICAL INDUSTRY TEAM PARTNERS MAP

Current partners of the CIT (CIT projects only) and commercialization partners are depicted below in Figure 3. These partners represent chemical companies, other industrial firms, national laboratories, universities, and other organizations.



Legend

□ ■ Chemical Companies ○ ● Industrial Firms ▭ Current CIT Partners
△ ▲ National Laboratories ☆ ★ Universities ▬ Partners in Commercialized Chemical Industry Projects
✚ Other

Figure 3. CIT Partners and Commercialization Partners

OIT Commercialized Chemical Industry Technologies

A number of technologies that are commercially available as a result of OIT support were developed by chemical company partners or have potential relevance to the chemical industry. These technologies are listed below. The remainder of this appendix contains brief descriptions of each of these technologies, along with OIT contacts.

Commercially Available Technologies Relevant to the Chemical Industry

- Arc Furnace Post-Combustion Lance
- Biphase Rotary Separator Turbine
- Catalytic Distillation
- Chemical Separation by Fluid Extraction
- Dual Cure Coatings
- Hydrochloric Acid Recovery System
- Hyperfiltration
- Membrane System for Purified Gas Production
- Methanol Recovery Process
- MotorMaster Software
- Oxygen-Enriched Combustion/Oxy-Fuel Firing
- Particle Size Distribution Sensor
- Plating Waste Concentrator
- Pinch Analysis and Industrial Heat Pumps
- Reclamation and Reuse of Wastewater
- Reverse Brayton Cycle Solvent Recovery Heat Pump
- Reversible Chemical Association Separation Technology
- Scrap Tire Recycling
- Solar Process Heat
- Solvent Recovery from Effluent Streams
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Arc Furnace Post-Combustion Lance [Contact: Scott Richlen, (202) 586-2078]
Steelmaking operations that use electric arc furnaces are applying the Arc Furnace Post-Combustion Lance technology to increase productivity, reduce energy requirements, and improve control. This technology was developed by a unit of Union Carbide, now part of Praxair, Inc., with support from both OIT and the American Iron and Steel Institute (AISI). It is currently in operation on electric arc furnaces at Nucor and Atlantic Steel, and is being marketed worldwide. The system consists of a water cooled lance and controls to inject oxygen to combust the carbon monoxide in and above the furnace's foamy slag. The result is a savings of 40-50 kilowatt-hours per ton of steel, and a 6-7% increase in productivity.

Biphase Rotary Separator Turbine [Contact: Pat Hoffman, (202) 586-6074]
The chemical and petroleum refining industries commonly recover the waste energy released when single-phase (all liquid or all vapor) process streams are depressurized. Thanks to a new turbine system developed with OIT support, much of the considerable energy released during the depressurization of biphase flows (consisting of both a liquid and a vapor) can now be recovered as well. The Biphase Rotary Separator Turbine, developed by Biphase Energy Systems, uses a nozzle to direct the two-phase mixture at high velocity against a rotating cylinder. Turning of the cylinder produces shaft power while the stream is simultaneously separated into liquid and gaseous phases for further processing and/or recovery.

Catalytic Distillation [Contact: Pat Hoffman, (202) 586-6074]
Distillation is one of the most energy-intensive industrial processes, accounting for over 40% of the energy consumed by the chemical industry each year. The single-stage, catalytic reaction/distillation process developed by Chemical Research and Licensing and OIT is being used to produce gasoline additives such as MTBE and TAME. Catalytic distillation saves energy by utilizing the heat released by the reaction to drive the distillation process, eliminating the need for a separate energy input. In addition, the conversion efficiency for production of MTBE or TAME is increased to over 99% from 97% for conventional processes. This technology is helping U.S. refiners produce the reformulated gasoline mandated by the Clean Air Act Amendments of 1990.

Chemical Separation by Fluid Extraction [Contact: Brian Volintine, (202) 586-1739]
With OIT support, CS Systems has developed an energy-efficient solvent extraction technology for removing hazardous organic compounds from contaminated soil or liquid waste streams, including industrial effluents. The technology uses a liquefied gas solvent (e.g., propane or carbon dioxide) to extract the contaminants from solids, sludges, and aqueous streams. Following extraction and separation, both the solvent and the extracted chemicals are recovered; the chemicals can then be recycled, reused, or disposed, and the residue, which is no longer hazardous, may be used as a process feedstock. The technology produces no harmful atmospheric emissions.

Dual Cure Coatings [Contact: Bruce Cranford, (202) 586-9496]
With OIT support, 3M has developed a low-VOC process for applying photo-cured, high-performance coatings that sacrifice nothing in terms of performance, appearance, or ease of application. The basis of this dual-cure process is a novel photocatalyst system that allows light-activated, simultaneous polymerization of two monomers to produce a material with two independent yet interpenetrating polymer networks. The process offers shorter cure times, flexibility in tailoring coatings for specific applications, and substantially lower VOC emissions than conventional methods. By using these new coatings, U.S. industry could reduce VOC emissions by an estimated 260,000 tons per year and save the energy that would otherwise have been used to dispose of VOC wastes and manufacture replacement solvents.

Hydrochloric Acid Recovery System [Contact: Alan Schroeder, (202) 586-1641]
To clean raw steel, galvanizing and other steel fabrication processors often use pickling -- immersion in a vat of hydrochloric acid (HCl). Although large installations have recycled used HCl for some time, recycling is now cost-effective for smaller facilities as the result of a new technology developed by Beta Control Systems through an OIT-supported project. This innovative, closed-loop technology uses an evaporator, absorption column, and stripper, along with the latest superplastics and electronic controls, to clean and concentrate the acid according to exact user specifications. The technology reduces the demand for virgin HCl acid, eliminates use of chemicals for neutralizing the waste acid, and saves energy in waste transport and disposal. The system gives small and medium-sized galvanizers (60% of the galvanizing industry) the potential to reduce spent HCl and neutralized sludge generation by 40,000 tons annually.

Hyperfiltration [Contact: Charles Russomanno, (202) 586-7543]
Hyperfiltration, a membrane-based separation technique originally developed for the desalination of seawater, has been adapted for treating industrial waste waters. With support from DOE, CARRE, Inc. (since sold to Graver Separations, Inc.) has developed the technology to process a wide variety of waste streams under a wide range of chemical conditions, pressures, and temperatures. Through the choice of renewable organic or inorganic membrane coatings, the technology achieves micro- to nano-level filtration to recover raw materials and minimize waste in the textiles, food processing, biotechnology, pharmaceuticals, pulp and paper, chemicals, electronics, and nuclear industries.

Membrane System for Purified Gas Production [Contact: Charles Russomanno, (202) 586-7543]
With OIT funding, A/G Technology has developed a hollow-fiber membrane system that improves the efficiency of combustion in industrial burners. Although ambient air contains 79% nitrogen and 21% oxygen, only the oxygen is used in the combustion process; heating the nitrogen represents a waste of energy. The semi-permeable, polymeric membrane system developed by A/G Technology increases the oxygen content of combustion air to about 35% and does so with less energy and at lower cost than other air separation processes. The compact membrane unit consists of thousands of hollow polymer fibers inside of a cartridge contained within a pressure vessel. It can be used to generate flow rates compatible with a wide range of industrial applications. Approximately 55 units are currently in use. A/G Technology has also adapted the system to produce purified nitrogen for other industrial applications.

Methanol Recovery Process [Contact: Alan Schroeder, (202) 586-1641]
The production of hydrogen peroxide involves the use of a catalyst that must be periodically regenerated by washing with methanol. In the process, the methanol becomes contaminated with organic solvents, hydrogen peroxide, and metal ions. With an OIT grant, FMC has equipped its facility in Pasadena, Texas, with a methanol recovery system based on steam distillation. This technology has achieved methanol recovery efficiencies close to 99% and prevents the build-up of potentially flammable or explosive contaminants, which can occur in the bottom of conventional distillation columns.

MotorMaster Software [Contact: Paul Scheihing, (202) 586-7234]
Three-phase electric motors and the systems they drive account for over 50% of all electricity consumed in the United States. Most high-efficiency motors repay their additional capital cost quickly in energy savings, but many potential users need help in finding the right motor for a particular application. To encourage the use of high-efficiency motors, OIT and the Bonneville Power Administration funded the development of the MotorMaster Software by the Washington State Energy Office. Updated twice yearly, the MotorMaster software contains performance and purchase information on about 10,000 currently available three-phase motors. Its review features include comparisons of efficiency, first cost, payback time, and operating cost. A new version of the software, MotorMaster Plus, may be used to track data such as energy and cost savings for each motor in a plant. The MotorMaster program is contributing to decreased energy use, reduced pollution from reduced demand for electric power generation, and lower operating costs to manufacturers and other users of electric motors.

Oxygen-Enriched Combustion/Oxy-Fuel Firing [Contact: Gideon Varga, (202) 586-0082]
OIT and Praxair, Inc., have demonstrated an oxygen-enriched combustion system for glass melting furnaces that significantly reduces melting energy requirements. Combustion using oxygen enriched air is more fuel-efficient than combustion using ambient air. The system uses an advanced oxygen supply system know as vacuum pressure swing adsorption, an energy efficient variation of conventional pressure swing adsorption technology. Approximately one-third of the 65 units currently in use are on smaller furnaces, where energy savings of up to 45% have been achieved. The remaining units are on larger furnaces, where energy savings have averaged about 15%. In addition, emissions of NO_x are reduced by up to 90%, carbon monoxide by up to 96%, and particulates by up to 30%.

Particle Size Distribution Sensor [Contact: Theodore Johnson, (202) 586-6937]
Slurries - mixtures of solids and liquids - are most commonly found in the chemicals, food processing, and pulp and paper industries. The lack of an effective method of measuring particle size distribution for slurries containing very small particles (less then 1 micrometer in diameter) at the high concentrations commonly found in industry is a major cause of overgrinding and low yield in the production of pigments, clays, and numerous other materials. Pen Kem, Inc., in cooperation with OIT, has developed a new sensor to measure particle size distribution in slurries. The sensor system uses a computer-based mathematical model to estimate particle size distribution from the behavior of ultrasound as it passes through a solid/liquid suspension of a given concentration. This technology reduces grinding electricity requirements and the production of substandard material. Five units have been sold to chemical companies and ceramics researchers.

Pinch Analysis and Industrial Heat Pumps [Contact: Paul Scheihing, (202) 586-7234]
The use of industrial heat pumps to recycle the waste heat currently being discarded can save energy while reducing combustion-related emissions. Pinch analysis can be used to optimize process heat integration and identify heat pump applications. Pinch analysis uses thermodynamics and engineering principles to track energy flows in a plant and identify where energy can be conserved for the least amount of money. Pinch analysis was performed in 14 plants representing the major process industries. Six of these plants proceeded with retrofit heat pump designs. A pinch analysis of a wet-corn-milling plant in Alabama showed that modifying the existing heat exchangers (evaporators) and adding a third heat pump to the existing heat pumps would save an additional 72 million Btu per hour, reducing overall process fuel use by as much as 33%.

Plating Waste Concentrator [Contact: Bruce Cranford, (202) 586-9496]
Electroplating and other industrial processes generate waste water with high concentrations of toxic heavy metals. Although these water pollutants represent lost chemicals, conventional recovery techniques are costly, energy-intensive, and result in a hazardous waste sludge. OIT therefore supported LICON, Inc. (now ALVAL International) in developing a low-cost vapor-recompression evaporation system for concentrating such waste water. The high-efficiency system employs a vapor-recompression evaporator complemented by a single-effect evaporator that uses the waste heat from the vapor leaving the evaporator.

Reclamation and Reuse of Wastewater [Contact: Alan Schroeder, (202) 586-1641]
With support from OIT, PPG Industries has developed a technology for reclaiming and reusing the contaminated waste water from water-based painting operations. After the contaminated water has been collected separately and pre-filtered to remove large solids, it is put through the ultrafiltration unit, where suspended solids and high-molecular-weight particles are removed. The smallest impurities are then removed by the reverse osmosis unit, and the water is pumped to a storage tank for later reuse in cleaning operations. The PPG facility using the system has reduced its annual tanker truck trips to a hazardous waste facility from 65 to 4, suggesting the technology's potential to achieve substantial energy savings and waste reduction throughout the coating industry.

Reverse Brayton Cycle Solvent Recovery Heat Pump [Contact: Paul Scheihing, (202) 586-7234]
Under an OIT contract, 3M and Nucon International developed a Brayton cycle heat pump that economically and efficiently recovers VOCs and other solvents from gaseous waste streams. The heat pump first condenses the solvent by compressing the solvent-laden gas stream and extracting heat from it at a constant pressure in a regenerator (the reverse part). The solvent stream then undergoes turboexpansion, which lowers the temperature and condenses the remaining solvent. Finally, the cold, solvent-free gases pass to the other side of the generator to recoup the heat. To further improve system economics, the pump can be integrated with a carbon adsorption/inert gas process to regenerate the adsorbent bed.

Reversible Chemical Association Separation Technology [Contact: David Boron, (202) 586-0080]
Through funding from OIT, the University of California at Berkeley and the Lawrence Berkeley National Laboratory developed a novel separation approach for extracting chemicals from industrial waste streams. The approach, which has been commercialized by Cargill, Inc., involves the use of an organic solvent or complexing agent to bind with chemical products in waste streams for simple separation and recovery. The technology eliminates the need for evaporation, the most energy-intensive alternative step. The initial application of the technology is the recovery of carboxylic acids (e.g., lactic acid and citric acid) from biomass and industrial waste streams.

Scrap Tire Recycling [Contact: Simon Friedrich, (202) 586-6759]
The 70 million scrap tires that go into stockpiles each year in the United States now have an additional avenue for conversion to good uses. OIT and Composite Particles, Inc. have developed a new surface treatment technology for finely ground tire rubber that allows it to be used in the manufacture of composites. The incorporation of surface-modified rubber particles increases the impact resistance and toughness of several types of coatings and paint, including epoxies, polyurethane, and latex systems. Using these particles in polyurethane in-line skate wheels greatly increases wheel traction on wet surfaces. A major manufacturer of skate wheels has developed a new line of such wheels that will be commercialized in the spring of 1997.

Solar Process Heat [Contact: Frank Wilkins, (202) 586-1684]
A large portion of the industrial sector's total energy consumption - 30% to 40% - is for process heating applications. Many of these applications can be met with solar process heat systems. Solar process heat systems convert solar radiation into heat. Most of the solar process heating systems use either flat plate or concentrating collector technology. In a flat plate system, the water to be heated is pumped through tubes that form the collector or are bonded to the plate. A concentrating collector focuses the incoming solar energy on a line or point to produce a concentrated heat source. OIT is working with the solar industry to establish a solid base of installed systems in niche markets, primarily the government and institutional sectors. A solar process hear system installed at the California Correctional Institution at Tehachapi provides hot water and uses 28,800 ft^2 of concentrating collectors to deliver 4.2 million Btu/hr (equivalent to 1,230 kW).

Solvent Recovery from Effluent Streams [Contact: Charles Russomanno, (202) 586-7543]
OIT and Membrane Technology and Research, Inc., have developed a membrane separation system for recovering VOCs and CFCs from producer and user air streams. The technology works by first compressing the contaminated air stream and then condensing it. After the condensed solvent has been collected for reuse, a highly selective membrane separates the gas mixture into an organic-enriched permeate stream and an organic-depleted stream. The former is recycled to the compressor, while the latter is vented. More than 40 VaporSep units have been installed to date.

Supercritical CO_2 Cleaning [Contact: Theodore Johnson, (202) 586-6937]
Supercritical fluids, particularly carbon dioxide (CO_2), have been identified as viable, environmentally benign alternatives to CFCs in the cleaning of organic and particulate contaminants from metals, plastics, electronic components, and other materials. The low operating temperatures and pressures of supercritical CO_2 systems reduce the energy required to "bake out" the cleaning solution from the treated part. The purchasing, treatment, and disposal costs associated with solvent use are also eliminated. OIT has formed a consortium of three national laboratories and numerous industrial firms to develop and evaluate supercritical cleaning technology for a variety of applications. Hughes Aircraft, for example, is commercializing it for dry cleaning applications.

Ultrasonic Tank Cleaning [Contact: Alan Schroeder, (202) 586-1641]
With funding from OIT, DuPont-Merck has developed a tubular, ultrasonic resonator that sends out energy waves in all directions at once to effectively clean even large tanks using just water and a little soap. The small unit can be placed in chemical and pharmaceutical tanks through the top openings, eliminating the need for workers to enter the tanks. By dispensing with the need for solvents, ultrasonic cleaning eliminates emissions of harmful VOCs and the generation of hazardous wastes. This technology cleans tanks more quickly and thoroughly than solvents, uses less energy, and reduces labor and material costs.

Variable Frequency Microwave Furnace [Contact: Charles Sorrell, (202) 586-1514]
Lambda Technologies used OIT funding to develop a variable-frequency microwave furnace that offers several benefits in a variety of materials processing operations. Whereas conventional microwave furnaces use standing waves that create non-uniform energy distribution in the working cavity, the new technology sweeps the frequency over a range so that the power distribution becomes uniform. Various polymer products can be uniformly cured in the new furnace, often in only 10% of the time required by traditional microwave furnaces. The new furnaces facilitate excellent process control at the molecular level, allowing new material structures not possible with conventional heating techniques.

VOC Control Assessment Software [Contact: Alan Schroeder, (202) 586-1641]
OIT has joined with the New York State Energy Office, the New York State Energy Research and Development Agency, and others to develop an innovative approach for recovering volatile organic compounds (VOCs) from industrial airstreams. The project has resulted in the development of computer software that identifies optimal VOC control strategies for individual facilities. Industry personnel can use the software on-site to help characterize the facility and its emissions and produce a list of least-cost options for controlling the VOCs.

VOC Recovery from Aqueous Waste Streams [Contact: Charles Russomanno, (202) 586-7543]
The manufacture of organic chemicals, plastics, synthetic fibers, pesticides, pharmaceuticals, and pulp and paper, together with the refining of petroleum, produce aqueous waste streams containing approximately 1.5 to 3 billion gallons per year of volatile organic compounds (VOCs). OIT and Membrane Technology and Research, Inc. have developed an energy-efficient membrane process (pervaporation) to recover VOCs from these waste streams for reuse in the generating process, as a raw material for other processes, or as a fuel. The technology has completed a year of successful commercial operation at one site and is being purchased for use by additional industrial firms.

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